Final
MODELING PROTOCOL

Development of Base Case Photochemical Modeling to Address 1-Hour and 8-Hour Ozone Attainment in the Dallas/Fort Worth Area

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1.0 INTRODUCTION

This document describes the procedures that will be used in the development of a new ozone-modeling database for the Dallas/Fort Worth (DFW) nonattainment area of Texas. A Modeling Protocol is needed whenever ozone modeling is carried out for the purpose of developing emission reduction strategies that may be included in a State Implementation Plan. The requirements for a Modeling Protocol are described in two U.S. Environmental Protection Agency (EPA) reports:

> Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS. EPA-454/R-99-004. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. May 1999
>
> Guideline for Regulatory Application of the Urban Airshed Model, EPA-450/4-91-013, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. July 1991.

A final version of the Draft Guidance is expected in mid-2003 and some changes are expected from the May 1999 version

1.1 BACKGROUND

The US Environmental Protection Agency (EPA) currently has a 1-hour ozone National Ambient Air Quality Standard (NAAQS) that simply stated, says no monitor can measure more than three exceedances (0.12 ppm or 124 ppb) in a three year period. With complete data capture compliance with the 1-hour ozone NAAQS requires that the fourth highest daily maximum 1-hour ozone concentration in three years at every ozone monitor in the area be less than or equal to 0.12 ppm. However, the standard is defined in terms of an expected exceedance rate (to compensate for inadequate data capture) that allows no more than one expected exceedance per year calculated over three consecutive years. Areas that have more than three exceedances violate the 1-hour ozone NAAQS and are classified as ozone nonattainment areas. Ozone nonattainment areas must develop an ozone emissions control plan and demonstrate that they will attain the ozone NAAQS by the date specified in the Clean Air Act Amendments (CAAA) in a State Implementation Plan (SIP). The SIP ozone attainment demonstration is usually accomplished using air quality modeling.

In 1997, EPA promulgated a new ozone NAAQS that is potentially much more stringent than the old 1-hour standard. The new form is based on ozone measurements averaged over eight hours; violations of the 8-hour ozone standard occur when the fourth highest 8-hour ozone concentration each year, averaged over three consecutive years, at an individual monitor exceeds 0.08 ppm (84 ppb). The actual nonattainment designations are likely to be based on ambient measurements taken during the three years between 2001-2003.

On May 14, 1999, the D.C. District Court declared that EPA exceeded their authority in setting the 8-hour ozone standard and remanded it back to EPA. EPA appealed the decision to the US Supreme Court who upheld the new 8-hour ozone standard in February 2001 but remanded implementation issues back to the lower court. The lower court issued a ruling in March 2002 that required EPA to develop a new 8-hour ozone implementation approach and EPA expects to propose such an implementation rulemaking soon. Although EPA has not officially proposed a new implementation schedule, it would likely require states to recommend to EPA their 8-hour ozone nonattainment areas and boundaries by mid-2003. EPA would likely then make 8-hour ozone nonattainment designations by April 2004 based on 2001-2003 ambient air quality data.

Previous Ozone Modeling Studies in the DFW Nonattainment Area

The 1990 Clean Air Act Amendments authorized the EPA to designate areas failing to meet the NAAQS for ozone as nonattainment and to classify them according to severity. The Dallas/Fort Worth area was classified a "moderate" nonattainment area and was required to demonstrate attainment by November 1996. A SIP was submitted with controls focused almost entirely on volatile organic compounds (VOCs); this SIP failed to help the DFW area reach national air quality standards by the deadline. As a result, the EPA reclassified the DFW area from "moderate" to "serious," resulting in a new attainment deadline of November 15, 1999.

The DFW area also failed to reach attainment by the November 1999 deadline. A new SIP was prepared based upon photochemical modeling for two episodes, June 20-22, 1995 and July 2-4, 1996. In April 2000, the TCEQ adopted a final attainment demonstration SIP based upon those episodes, which asserted the importance of local NOx reductions as well as the transport of ozone and its precursors from the Houston/Galveston area. Based on additional photochemical modeling demonstrating transport from Houston/Galveston, the agency requested an extension of the DFW attainment date to November 15, 2007, the same attainment date as for Houston/Galveston.

During this period, federal lawsuits were filed challenging extensions to attainment dates based upon transport. The courts have determined that the Clean Air Act Amendments do not give the EPA authority to grant extensions to the 1-hour attainment dates. Therefore, EPA has not approved the most recent DFW SIP, and is currently evaluating its options with regards to reclassification. If the DFW area is reclassified again, a new SIP will need to be prepared within a year of redesignation.

Purpose and Objectives

Given the short time available until a new SIP must be submitted, DFW and the state of Texas will need to move quickly to develop the emissions and photochemical modeling databases needed to develop 1-hour and 8-hour ozone plans by 2004. The first step in the development of a photochemical modeling database for SIP planning is the development of a Modeling Protocol (this document) that conforms to the requirements in the EPA guidance documents

(EPA, 1991, 1999). The key objectives in developing an all-new photochemical modeling database for the DFW area are as follows:

- To select representative 1-hour and 8-hour ozone modeling episode(s) for the 4-county Dallas/Fort Worth Nonattainment area.;

- To create a photochemical modeling domain consistent with the Texas standard domain using a Lambert Conformal Projection (LCP) to be consistent with the MM5 meteorological model. The coarse grid domain must be sufficiently large to treat multi-day transport of ozone and precursors from significant source areas outside of Texas ;

- To create a nested-grid with 4-km grid spacing large enough to include the DFW 4-county nonattainment area as well as the 8 surrounding counties that constitute the Consolidated Metropolitan Statistical area. All nested grids will telescope at a 3:1 ratio (e.g., 36, 12, 4-km) to be compatible with the MM5 meteorological modeling grid system;

- To produce refined meteorological inputs for the entire domain using version 3 of the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5), while optimizing performance in the fine-grid DFW subdomain containing the DFW CMSA.;

- To incorporate the latest available emissions data for Texas as well as other areas within the regional-scale grid domain;

- To create a Comprehensive Air Quality Model with extensions (CAMx) Base Case simulation of the selected episode, including diagnostic tests, performance evaluation, and basic sensitivity analyses to provide directional guidance for follow on work;

- To perform Base Case VOC/NOx emissions reduction sensitivity tests and estimate appropriate near term categorical control strategies under different VOC/NOx emission reduction regimes; and

- To provide the CAMx modeling database, pre- and post-processor systems, display programs, and other data and programs developed to meet these objectives to the TCEQ staff, the EPA, designated representatives from the DFW area, and other interested parties.

It should be noted that the current activities undertaken as outlined in this Modeling Protocol do not include future case control strategy evaluation. However, this protocol assumes that all planned regional controls in effect at the time of the August 1999 episode (e.g., Tier 2/Low Sulfur and Heavy Duty Diesel on-road mobile source rules) and local Texas controls (e.g., DFW, HGA, Northeast Texas ozone control plans) will be included in the base case modeling.

1.2 SCHEDULE AND DELIVERABLES

The schedule of activities currently planned under the DFW ozone modeling study is shown in Table 1-1. This schedule is subject to revision, based on any changes that may occur in the technical direction as directed by the State, including any revision of objectives or requirements for the study. The modeling plan and schedule may also need revision after EPA announces their 1-hour bump-up procedures, attainment deadlines and any revisions to the 8-hour ozone implementation policy.

Table 1-1. Schedule for Dallas/Fort Worth 1999 base case ozone modeling activities.

Task	Completion Date
Modeling Protocol Development	May 2003
Meteorological Modeling	April –May 2003
Emissions Modeling	April - May 2003
CAMx Air Quality Modeling	June - July 2003
Final report	July 2003

An interim report will be prepared for each of the major tasks listed in Table 1-1, and submitted to State and local representatives after the completion of each task. The reports will include the following:

- A draft Modeling Protocol will be submitted to the state and local agencies. After receiving comments on the draft Modeling Protocol, a draft final Modeling Protocol will be submitted. Note that any Modeling Protocol is a “living document’ which evolves over time as the modeling proceeds and scientific judgement and professional interpretation are applied to the model results. Normally this evolution results in minor changes to procedures and adjustments to model inputs which occur frequently enough that formal updates to the modeling protocol are impractical. Therefore these changes are documented in the task reports which are submitted at each stage of the modeling process. If significant changes or revisions are required, the TCEQ will work closely with EPA Region VI and with DFW stakeholder groups to justify and explain the changes.

- A draft report describing the MM5 meteorological modeling, including data sources, modeling methodology, and performance evaluation, will be submitted to the State and local agencies. CAMx-ready meteorological input files will be made available on an FTP site. We will compile a tape archive of the MM5 input and output data for subsequent distribution to the State and local agencies.

- A draft report fully documenting the emissions data, methodologies and results will be submitted to the State and distributed among local agencies. The draft report will include an emissions quality and reliability assessment, and the inventories developed under this task will include all updates identified by the State with input from local agencies as a result of the quality and reliability assessment. The "CAMx-ready" base year emission inventories, models, run scripts and final outputs will be made available on an FTP site for download by interested parties.

- A draft report describing the CAMx Base Case modeling, including methodology, performance evaluation, base case animations and a full description of all sensitivity/diagnostic applications will be submitted to the State and distributed among local agencies. The CAMx modeling database will be made available on an FTP site. We also propose to compile a tape archive of the CAMx input and output data for subsequent distribution to the State and local agencies that may then provide it to any project participants who request it.

1.3 STUDY PARTICIPANTS

Contractors

The modeling for this study is being performed by ENVIRON International Corporation (ENVIRON). The key personnel at ENVIRON who are directing and performing the study are identified below along with their contact information:

Dr. Greg Yarwood	Principal Investigator	415/899-0704	gyarwood@environcorp.com
Dr. Gerard Mansell	Project Manager	415/899-0727	gmansell@environcorp.com
Mr. Chris Emery	Meteorological Modeling	415/899-0740	cemery@environcorp.com
Ms. Michele Jimenez	Emissions Modeling	415/899-0734	mjimenez@environcorp.com

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Policy Group and Technical Advisory Committee

The Texas Commission on Environmental Quality (TCEQ) will administer the contract with ENVIRON and act as a managing body for the project. Representatives from the various local agencies, as well as from the TCEQ and EPA, will provide technical information where needed and will oversee and review all work performed in this project. The individuals comprising the Policy Group and DFW Photochemical Modeling Technical Committee s are shown in Table 1-2.

Table 1-2. Participants in the Dallas/FortWorth Photochemical Modeling Technical Committee.

DFW Photochemical Modeling Technical Committee Members

NAME	REPRESENTING
Alvarez, Ramon	Environmental Defense
Barnes, Paul	The Pilot Group, Inc.
Blackmon, Linden	Mrs. Baird's Bakeries
Bornhorst, Becky	Downwinders At Risk
Burnam, Earl	Tarrant Coalition for Environmental Awareness
Dai, Weiping	Trinity Consultants
Dawson, Harold	City of Garland
DePalma, Deena	DFW Airport
Dharmarajan, N.N.	American Electric Power
Diggs, Tom	EPA - Region 6
Duncan, David	TXU Energy
Escobedo, Carmen	City of Grand Prarie
Floyd, Mark	Air Force Reserve Command
Frigs, Hendrik	Self
Grossman, David	The Pilot Group, Inc.
Gunzelman, Brian	Shaw Environmental
Hatfield, Tom	City of Richardson
Hohman, Bob	City of Irving
Hubener, Katy	Blue Skies Alliance
Johnson, Rita	AAA Texas
Larsen, Alan	Raytheon Systems Co.
Mason, Eric	City of Fort Worth
McHugh, Simon	Associated General Contractors of America, Inc.
Mendias, Michael	Vought Aircraft Industries, Inc.
Michael, T.C.	City of Fort Worth
Miller, David	City of Dallas
Morris, Shannon	North Texas Clean Air Coalition

NAME	REPRESENTING
Musgrove, Martha	Fort Worth Transportation Authority
Nelson, Phyllis	City of Dallas
Nguyen, Quang	EPA Region 6
Oliver, Timothy	Tetra Tech EM, Inc.
Pinto, Francisco	North Texas Cement
Robertson, Dick	TXU Energy
Rosenthal, William	Lockheed Martin
Savage, David	Baker & Botts, L.L.P.
Savoie, Spencer	General Motors
Schermbeck, Jim	Downwinders At Risk
Scott, Bob	Tarrant Coalition for Environmental Awareness
Sherrow, Herb	EPA Region 6
Smith, Tom (Smitty)	Public Citizen
Snyder, Erik	EPA Region 6
Stewart, Robert	Baker & Botts, L.L.P.
Turner, Usha	TXU Energy
Uphoff, Irvin	Self
Zarubiak, Darcey	DFW Airport
Zimmermann, Keith	RMT, Inc.

2.0 EPISODE SELECTION

2.1 EPA's GUIDANCE FOR EPISODE SELECTION

The modeling planned in this protocol must address both the requirements for1-hour attainment demonstrations as well as look ahead toward an 8-hour attainment demonstration for the Dallas-Fort Worth (DFW) area. There has been considerable evolution in the EPA procedures since the 1-hour demonstration requirements were first promulgated. As a result, this protocol refers frequently to the more recent conceptualizations of 1-hour and 8-hour ozone analysis procedures and the evolving 8-hour attainment demonstration procedures as proposed by the EPA.

EPA's draft 8-hour ozone modeling guidance has four primary criteria for selecting meteorological episodes for 8-hour ozone attainment demonstration modeling (EPA, 1999):

1. Select a mix of episodes that reflect a variety of meteorological conditions that frequently correspond with observed 8-hour daily maximum ozone concentrations > 84 ppb at different monitoring sites;
2. Select periods during which observed 8-hour ozone concentrations are close to the 8-hour ozone Design Value (i.e., three-year average of fourth highest 8-hour ozone concentration) at each key monitor;
3. Select periods for which extensive air quality/meteorological databases exist; and
4. Model sufficient number of days so that the model attainment test can be applied at all of the key ozone monitoring sites.

As noted in the draft EPA guidance, these four criteria may conflict with each other, and there may be other secondary criteria that can be used in the episode selection:

- Prior experience modeling an episode may result in it being chosen over an alternative;
- Choosing episodes corresponding to the three-year period being used to make the 8-hour ozone attainment designation may be desirable;
- May want to choose a modeling period in which days have 8-hour ozone concentrations near the 8-hour ozone Design Values at all violating monitors;
- If observed 8-hour ozone exceedances occur on weekends, weekend days should be considered; or
- If multiple areas are being modeled, then episodes that have 8-hour ozone exceedances in other areas may be considered.

The latest national emissions inventory information is from the 1999 National Emissions Inventory (NEI99). The next national emissions inventory update will be in 2002. This national inventory would likely be available in early 2004. In discussions with EPA on 8-hour ozone modeling they noted that they would prefer episodes from 1999 to present. Thus, we focused our episode selection procedures on episodes that occurred between 1999 and 2002.

2.2 PROCEDURES FOR EPISODE SELECTION

In the fall of 2002, ENVIRON, under contract to the TCEQ, developed a revised conceptual model of ozone formation in the DFW ozone non-attainment area. Following EPA's guidelines, candidate modeling episodes were identified and analyzed for use in attainment demonstration for the DFW area. The development of the conceptual model for ozone formation involved the compilation and analyses of various data regarding air quality, emissions and meteorology. In particular, the following analyses were included in the assessment:

- Ozone and air quality trends. Trends in ozone air quality within the DFW nonattainment region were considered. Both the ozone design values and Air Quality Index were evaluated with respect to variations from year to year and over the past 25 years. Comparisons with other nonattainment areas within Texas were also conducted. One-hour and eight-hour ozone exceedances were examined within the area to determine the frequency of exceedances during various time periods.
- Emission inventory trends. Trends in emissions of NOx and VOC were evaluated within the DFW area. The relationship between emission reductions from 1990 to 2001 and ozone air quality were considered. Comparisons with other nonattainment regions in Texas were also examined. These relations provide insight into the relative improvements in air quality and emission reduction strategies with respect to attainment of the NAAQS.
- Meteorological factors associated with high ozone events. The meteorological factors associated with high (and low) ozone events in the DFW area were evaluated. Surface winds provide an indication of the importance of local emission sources on air quality while upper level, or transport, winds reveal the influence of regional scale emissions and air quality. Evaluation of the general synoptic and mesoscale meteorological factors associated with ozone exceedances provide some guidelines for selection of appropriate episodes for further analysis and possible air quality modeling
- Episode selection. The development of the conceptual model provides the basis for the selection of representative modeling episodes required to demonstrate attainment of the ozone NAAQS. Based on the analysis conducted as part of the model development, several candidate episodes were identified.
- EPA Guidance documents. The EPA has developed guidance documents for evaluating and selecting modeling episodes for demonstration of attainment of both the 1-hour and 8-hour ozone standards. These guidance documents and the recommendations therein provide a basis for the selection of candidate episodes for the DFW nonattainment area.

The development of the conceptual model of ozone formation in the DFW non-attainment area is documented in detail in ENVIRON (2002). A summary of the more salient features of the conceptual model is presented in the following sections.

2.3 1-HOUR AND 8-HOUR OZONE TRENDS IN THE DFW NONATTAINMENT AREA

The development of the conceptual model for the Dallas/Fort Worth metropolitan region evaluated ozone trends for the years 1971 through 2001. The model looked at trends in ozone design values as well as ozone exceedances. Geographical patterns associated with elevated ozone levels were also considered, as were trends associated with particular years, months of the year, day of the week and time of day.

Ozone Levels and Design Value Trends

The 1-hour design value is determined by evaluating the fourth highest monitored ozone concentration in the most recent three years. The design value is calculated for each monitor, and the highest individual design value determines the design value for the non-attainment area.. The 8-hour ozone design value for an individual monitor is defined as the fourth highest monitored 8-hour ozone value averaged over the most recent three years of data. The design values provide an indication of the ozone air quality in the area and can be used to gauge an area's progress towards meeting the NAAQS for ozone. As part of the development of a conceptual model for DFW design value trends were examined. Design value trends for individual monitors as well as for the nonattainment area as a whole were evaluated for various time periods. Both the 1-hour and 8-hour design values were considered. Figure 2-1 displays the location of ozone monitors within the DFW nonattainment area. In recent years, the highest design values for the area have been established at sites on the North and West side of the DFW area.

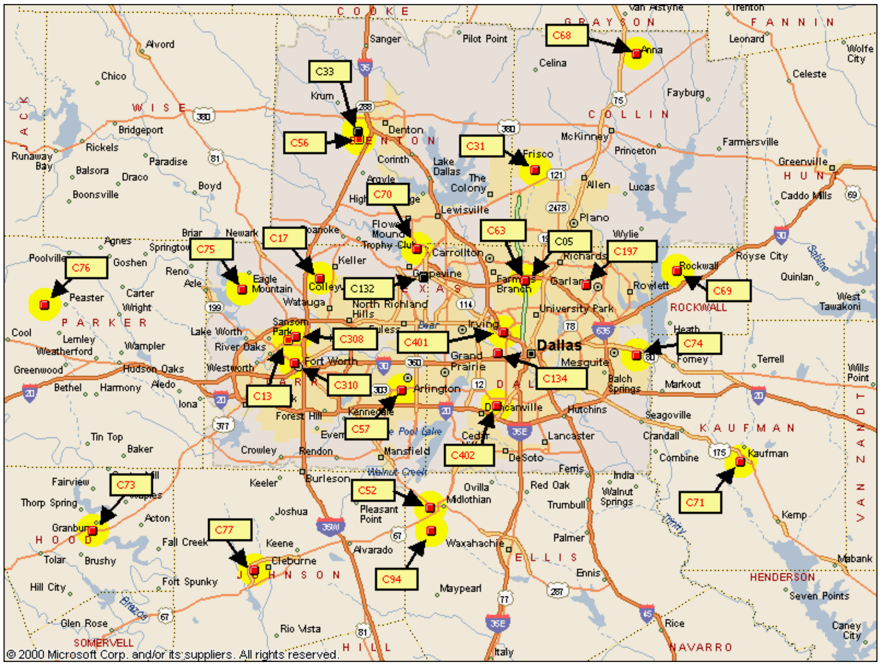


Figure 2-1. TCEQ monitoring site locations in the DFW area.

The DFW 1-hour ozone area maximum design value trend for the period 1974 through 2001 is displayed in Figure 2-2. Figure 2-3 displays the DFW 1-hour design values for each individual monitor. Examination of the trends displayed in Figures 2-2 and 2-3 reveal an overall consistent downward trend in the 1-hour design values during the period 1974 through 1988.

During the years 1988 through 2001 the 1-hour design value remained essentially unchanged at a value of approximately 140 ppb, which exceeds the federal one-hour ozone standard. The DFW 1-hour design value is currently at 137 ppb, having dropped to a minimum value of approximately 130 ppb in 2000.

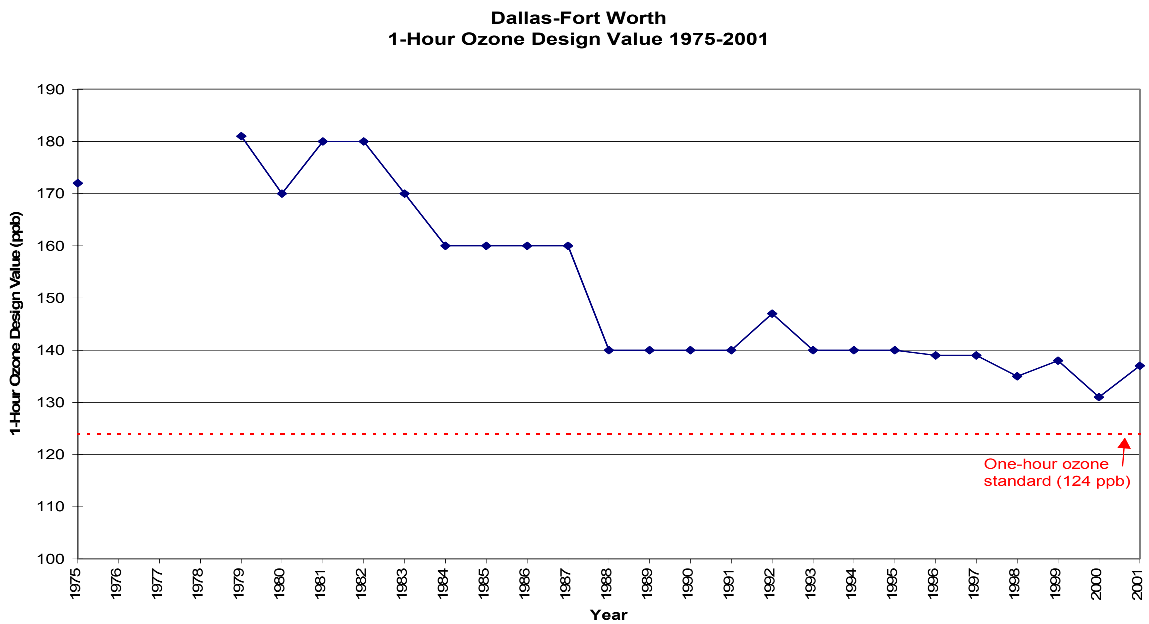


Figure 2-2. DFW 1-hour ozone design value trend for 1974-2001.

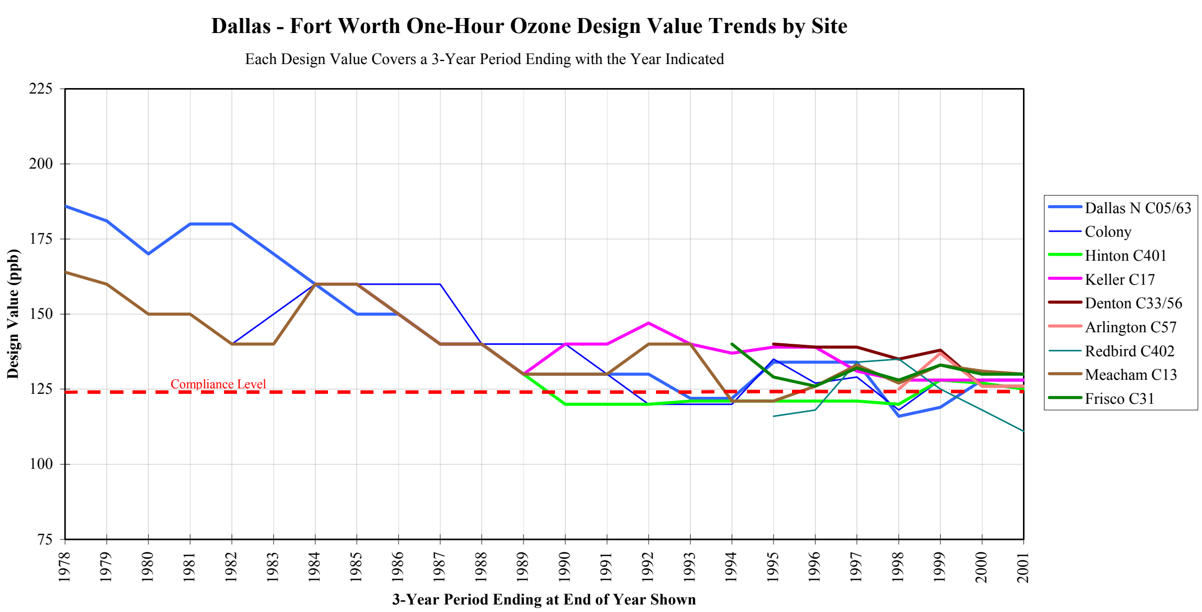


Figure 2-3. DFW 1-hour ozone design values by monitor for 1974-2001.

Examination of the design values for individual monitors (Fig 2-3) reveals the effects on the overall trends of the introduction of new monitors through time. The increase in 1-hour DFW area design value seen in 1992 can be seen to be due to the measurement at the Keller (C17) monitor, which came on-line in 1989. Likewise, exceedances recorded at other new monitors that began operation in the late 1990's contribute to the maintaining the design value at, or near, the level of 1993, of approximately 140 ppb. Preliminary assessment of 2002 data indicate that the 1-hour design value for the DFW area is now 136 ppb established at the Keller monitor (C17).

The 8-hour ozone design value for Dallas/Fort Worth, displayed in Figure 2-4, likewise shows an overall downward trend during the period 1974 through 1994, when the value again increases slightly to the 2001 design value of 101 ppb. Preliminary analysis of 2002 indicates that the 8-hour design value for the DFW area should now be 99 ppb, established at the Denton monitor (C56). An analysis of the data presented in Figure 2-5, which displays the 8-hour design values for individual monitors over the period from 1971 through 2001, again reveals the influence of new monitoring stations on the region-wide design values.

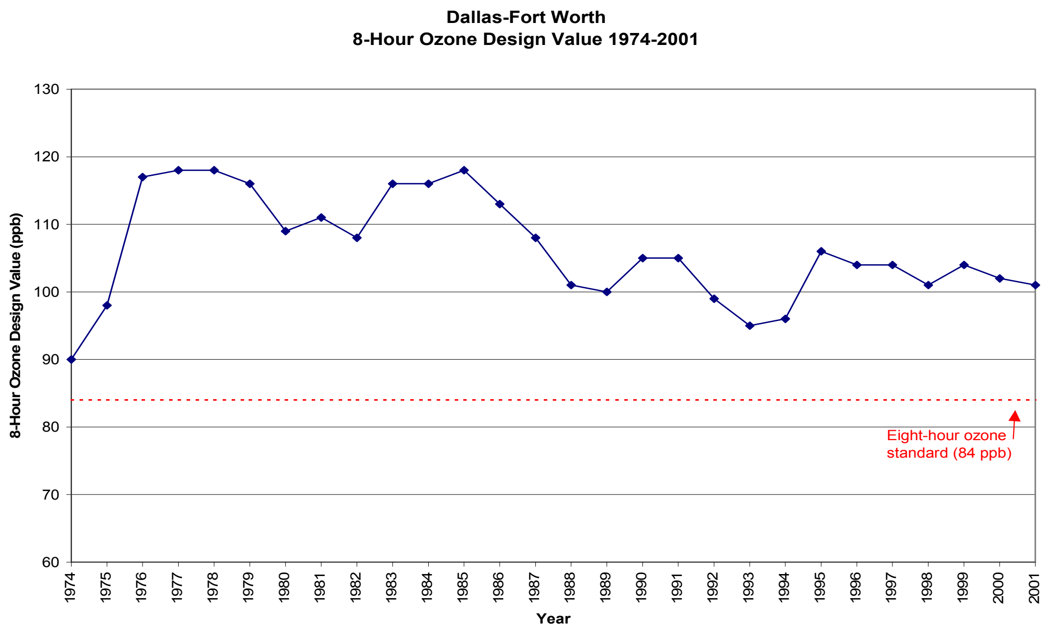


Figure 2-4. DFW 8-hour ozone design value trends for 1974-2001.

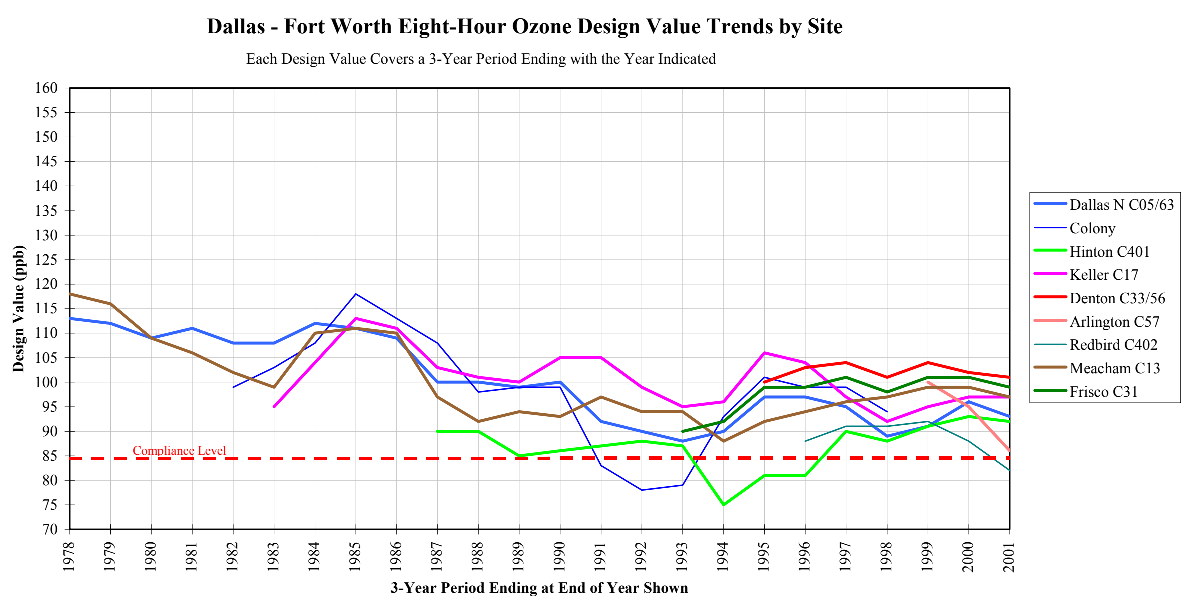


Figure 2-5. DFW 8-hour ozone design values by monitor for 1974-2001.

The overall downward trend in observed design values and the associated improvements in air quality are the result of several factors. The implementation of mobile source control programs and the replacement of older, carbureted motor vehicles with a pool of newer, more tightly controlled vehicles are significant contributors to improvements in ozone air quality. This conclusion however depends on whether VOC or NOx levels are more important. Although the flattening of the 1-hour design value trend line in recent years may reflect the transition to a newer, cleaner vehicle fleet, the overall balance in the situation is probably more complicated.

In recent years the design value has remained nearly constant in spite of the dramatic increase in the level of construction and economic activity. Over the same period, VMT growth has been outweighing emission factor reductions due to the cleaner fleet. So, while the long term downward trend in design values is encouraging, and suggests that existing controls may be sufficient to maintain the 1-hour ozone standard, the recent flattening suggests that additional controls will probably be necessary to attain the more stringent 8-hour NAAQS.

Ozone Exceedance Trends

The ozone season in the Dallas/Fort Worth area is typically eight months long, lasting from March through October and often exhibits two distinct peaks; one in late June/early July and one in late August. The mid summer lull between the peaks occurs at slightly different times each year, so it may be obscured when multi-year data is smoothed over longer time periods. However, the lull and the double peaks are apparent when the data from individual years is reviewed.

Figure 2-6 displays the number of 1-hour ozone exceedance days in the DFW nonattainment area during the years 1974 through 2001. Over the entire period, 1-hour exceedances decreased from 17 days to 2 days per year. However, exceedances during the more recent 1990 through 2001 period vary considerably each year ranging from 2 to 7 days per year. So while an overall downward trend is evident over the entire 1974-2001 time period, the analysis of ozone exceedances from the more recent 1990-2001 period does not indicate any clear trend.

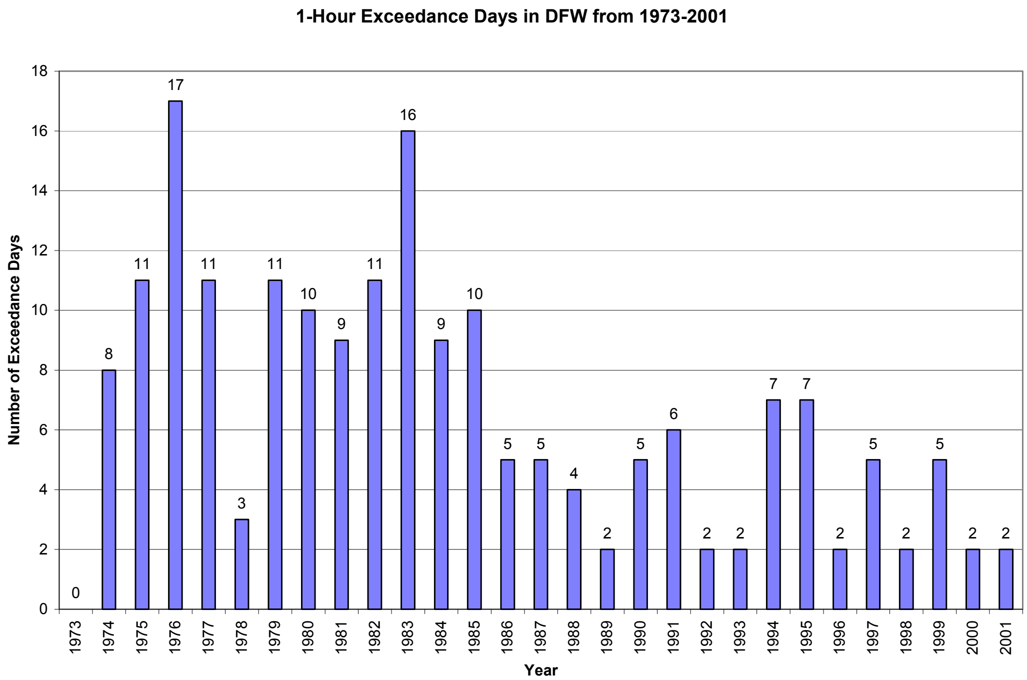


Figure 2-6. Number of 1-hour ozone exceedance days in DFW by year from 1974-2001.

The numbers of 8-hour ozone exceedance days in DFW over time are displayed in Figure 2-7. Data evaluated for the 8-hour ozone exceedances included only the years 1997 through 2002, and only the primary ozone season months (June-September). No clear trend can be seen in the data. Exceedance days range from 28 days per year in 2001 to 35 days per year in 1999, many more than appear in the 1-hour record. There does not appear to be any overall improvement in 8-hour exceedances during this relatively short time period.

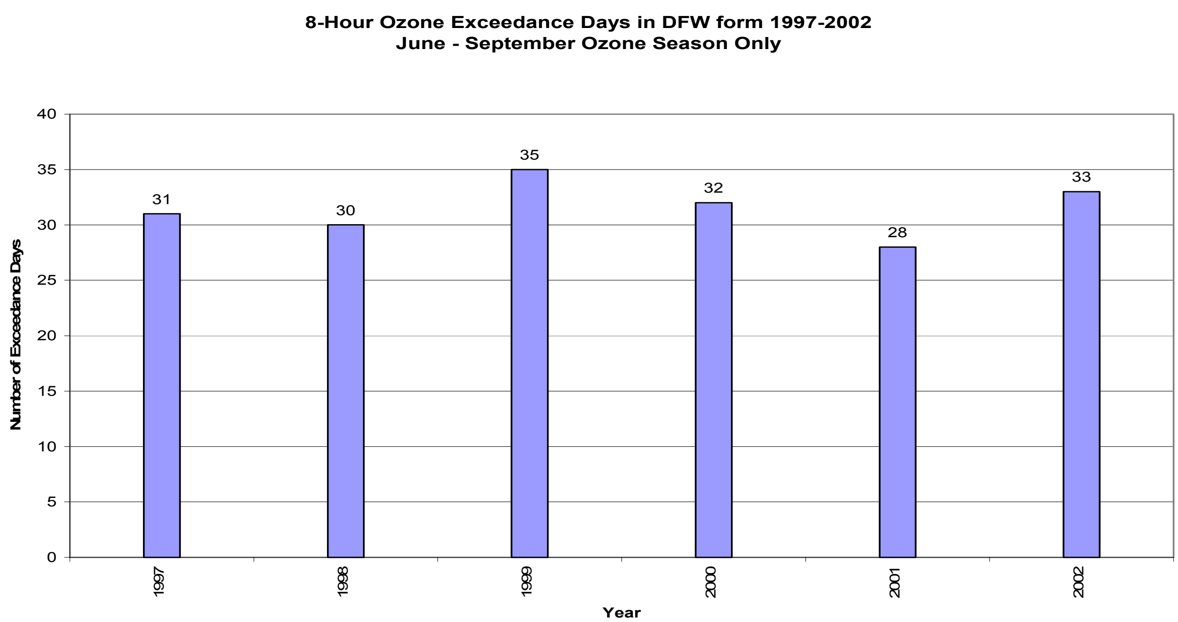


Figure 2-7. Number of 8-hour ozone exceedance days in DFW by year from 1997-2002 (June-September months only).

Consideration of the number of exceedance days by month-of-year (Fig 2-15) clearly indicates that the peak ozone season occurs during mid summer with the most 1-hour ozone exceedances occurring during the month of August followed by the month of July. These statistics are based on evaluation of ozone monitor data from the years 1997 through 2001. A previous analysis conducted by the TCEQ on data over 11 years from 1990-2001 indicates the same conclusions regarding the frequency of exceedances by month of year. Figure 2-8 present the 1-hour data from the more recent, shorter period.

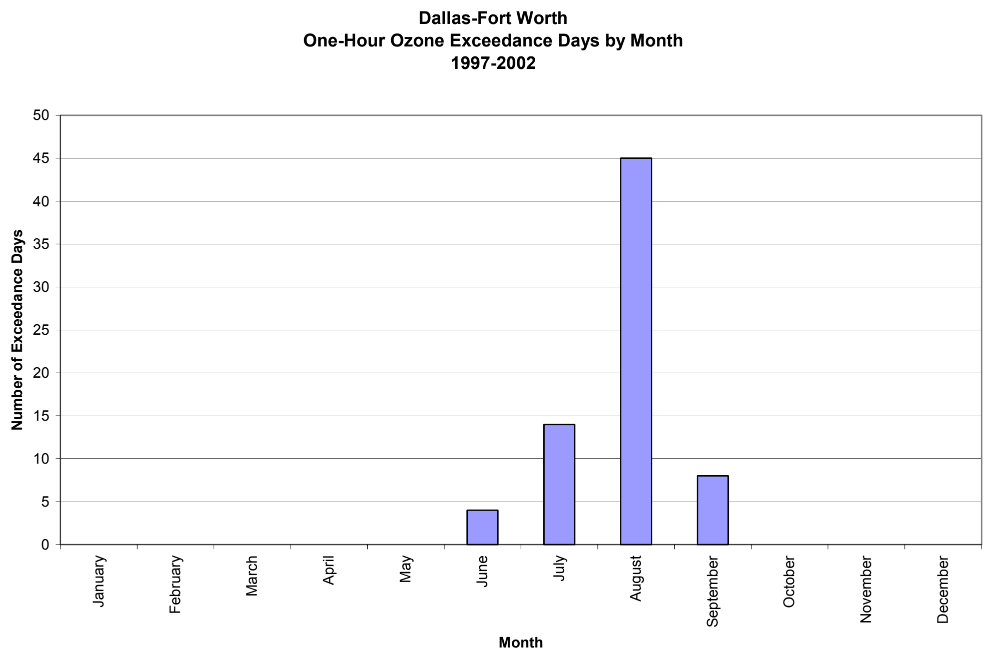


Figure 2-8. Number of 1-hour ozone exceedance days in DFW by month from 1997-2002.

Eight-hour ozone exceedance days by month of year are presented in Figure 2-9 for the years 1997 through 2002. As with the exceedance days by year, only the months of June through September were evaluated. As shown, the highest number of 8-hour ozone exceedances again occurs during the month of August, but followed by September in the 8-hour case.

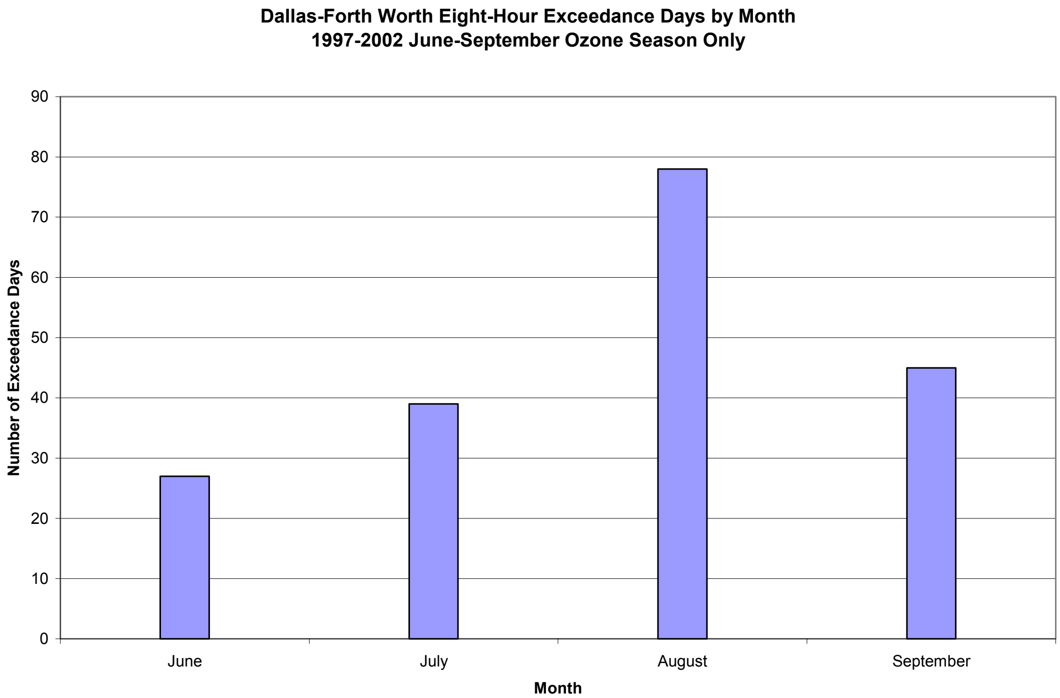


Figure 2-9. Number of 8-hour ozone exceedance days in DFW by month from 1997-2002 (June-September only).

2.4 EMISSION TRENDS AND INVENTORIES

An analysis of emission sources and trends is an important component of conceptual models of ozone formation. The relationship between ozone precursor emissions and ozone exceedances within the region can provide an indication of the efficacy of existing local controls, while an evaluation of regional emission inventories and trends provides a measure of the impact of upwind sources and long-range transport on high ozone events within the local region of interest.

As part of the development of the conceptual model for the Dallas/Fort Worth non-attainment area, trends in emission levels of volatile organic compounds (VOC) and oxides of nitrogen (NOx) were evaluated. The primary source categories contributing to the emission totals in the region include point, area, non-road mobile and on-road mobile sources.

NOx and VOC emission trends were evaluated for the DFW metropolitan area. Trends data for 1990 through 2001 as developed by ENVIRON for area and mobile (on-road and off-road) source categories (ENVIRON, 2001) for all Texas counties were evaluated. Point source emissions data were obtained from the TCEQ's Point Source Data Base (PSDB) system for the Dallas/Fort Worth, Beaumont/Port Arthur and Houston/Galveston nonattainment areas for the years 1992 through 2001. Emission estimates by county for the DFW and BPA areas for 1996 were also available from the TCEQ for evaluation as were 1999 region-wide emission totals for the nonattainment areas. The EPA's NEI99 version 2 was also examined to determine overall trends by county and region for 1999.

Figures 2-10 and 2-11 display the total annual anthropogenic VOC and NOx emissions for the Dallas/Fort Worth area for the years 1990 through 2001, respectively. Also shown for comparison are total anthropogenic NOx and VOC emissions for the Beaumont/Port Arthur and Houston/Galveston nonattainment area. Total annual emissions of these pollutants across all source categories in the DFW region have decreased over the past decade from 225,058 tpy NOx and 211,805 tpy VOC to 186,682 tpy NOx and 142,605 tpy VOC.

Based on TCEQ data, total NOx emissions in DFW decreased by approximately 10% from 1996 (186,855 tpy) to 1999 (167,195 tpy). During the same period, total VOC emissions decreased by approximately 23 % from 165,401tpy in 1996 to 127,294 tpy in 1999, based on data presented by the TCEQ (TCEQ, 2002a). Although these reductions in total emission are considerable, there appears to be no corresponding decrease in the ozone design values for this time period.

A previous analysis of emission trends in the DFW area considered emission data over the period 1985-86 to 1995-96 (TCEQ, 2002a). VOC data collected during this period showed a statistically significant downward trend, with an overall reduction of approximately 62%. The analysis indicated the same downward trend when only high ozone days were considered. The conclusion was that over the past 15 years, federal and state controls, particularly on motor vehicles, have been effective in reducing emission levels of one of the ozone precursors within the DFW metropolitan area. Similar conclusions may also be made from the data analysis considered here.

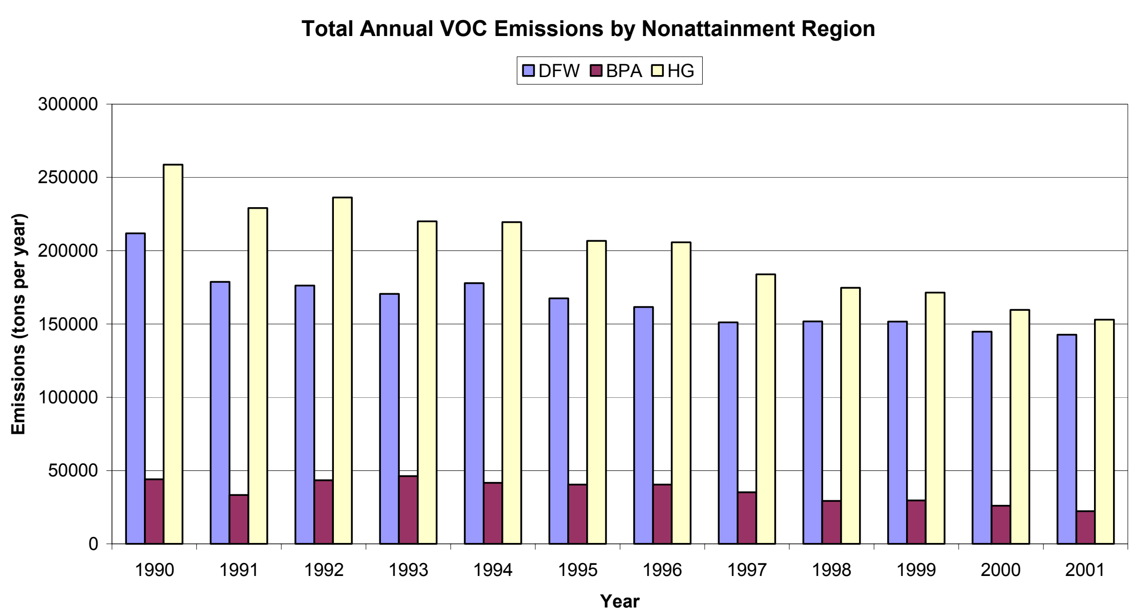


Figure 2-10. Total annual VOC emissions by nonattainment region from 1990-2001.

The TCEQ study also evaluated NOx emission levels over this same period (1985-86 to 1995-96) and noted an initial decrease followed by a subsequent increase of NOx emissions within the region. These overall decreases were attributed to increases in VMT in Dallas/Fort Worth. Although these trends were not considered statistically significant, the 1998-1999 increase supports the need for a NOx oriented strategy to control ozone levels in the DFW area.

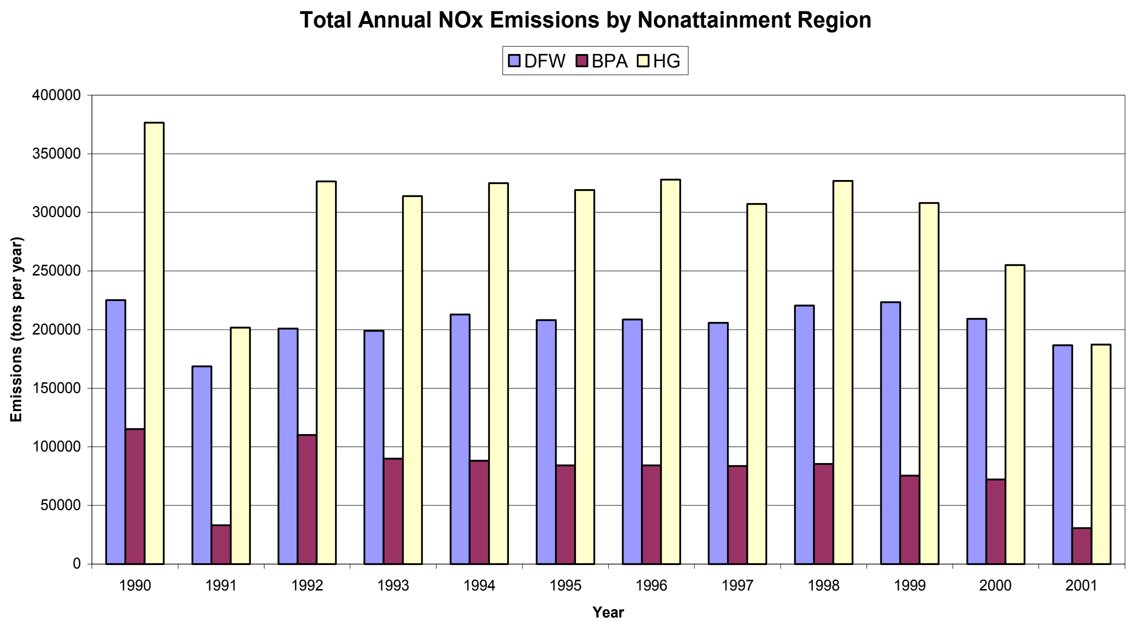


Figure 2-11. Total annual NOx emissions by nonattainment region from 1990-2001.

2.5 METEOROLOGICAL FACTORS

The DFW conceptual model considered the meteorological factors associated with both low and high ozone days within the region. Upper level, or transport winds, as well as surface wind flows were evaluated. In general, low ozone days are associated with relatively strong southerly wind flows. In contrast, the flow associated with high ozone days can be characterized as light winds from the southwest in the morning, shifting to light winds from the southeast in the afternoon. The analysis of transport level winds also suggests evidence of transport of ozone and ozone precursors from south and south central Texas. Evidence of transport between Dallas and Fort Worth was also noted, and will be discussed below. Thus, the ozone air quality in the DFW region is affected both by local sources as well as regional transport.

Local Meteorology

The Dallas/Fort Worth metropolitan area is located on the plains of Northeast Texas where the lack of major geographic features means that wind patterns are driven primarily by synoptic scale meteorological influences. Nonetheless, an analysis of local surface winds provides an understanding of the effects of local transport on ozone levels within the DFW urban area and can provide evidence of transport between Dallas and Fort Worth.

An analysis of surface wind trajectories was conducted by the TCEQ (TCEQ, 2002a; 2002b). The analysis examined local wind patterns for both high ($O3 > 125$ ppb) and low ($O3 < 80$ ppb) ozone days. Wind rose analyses were conducted which considered surface wind speeds and directions on high and low ozone days during the period 1990 through 2001. The analysis was conducted separately for both morning and afternoon hours. Displays of wind roses for Dallas and Fort Worth separately for morning and afternoon surface winds are displayed in Figure 2-12 through Figure 2-15.

The conclusions reached from these analyses can be summarized as follows. On low ozone days, the surface wind speeds tend to be relatively high compared to high ozone days. The winds generally blow from the south during both morning and afternoon. These wind speeds and directions are similar for both Dallas and Fort Worth. The relatively high wind speeds tend to ventilate the area of ozone and ozone precursors, limiting the potential for high ozone buildup.

By contrast, on high ozone days, the predominant wind directions are from the south and south-southwest with relatively low speeds. In the morning hours, Dallas surface winds tend to blow from the south-southwest shifting to the South and south-southeast during the afternoon.

Winds from the north are relatively rare during the ozone season in both Dallas and Fort Worth. In Fort Worth, high ozone days experience low wind speeds, with generally more random directions although an easterly wind component is present in the morning hours. The afternoons on high ozone days experience a more pronounced easterly component in surface winds compared to morning winds.

A comparison of surface winds on high ozone versus low ozone days reveals that winds on high ozone days tend to be lighter than on low ozone days, with calm winds much more frequent, increasing from approximately 2.6% to 17.3% of the time during the morning hours for Dallas. In Fort Worth calm morning winds occur approximately 1.8 percent of the time increasing to 12.9 % on high ozone days. High ozone days also exhibit more variation in wind direction, with morning winds blowing from the South-Southwest and afternoon winds shifting to the South-Southeast.

Meteorological conditions associated with the above situation provide evidence for local transport of ozone between Dallas and Fort Worth. Low wind speeds in the morning hours allow for accumulation of precursors and ozone production in the urban areas. The easterly wind directions in Fort Worth during the morning hours may transport ozone and ozone precursors from Dallas. Likewise, the westerly winds in Dallas may lead to transport of ozone and precursors from Fort Worth. The relatively low wind speeds on high ozone days cause ozone levels to build up. The shift in wind direction in the afternoon then leads to transport of elevated ozone levels from Dallas back to Fort Worth.

High Ozone (O3 > 125) for Dallas

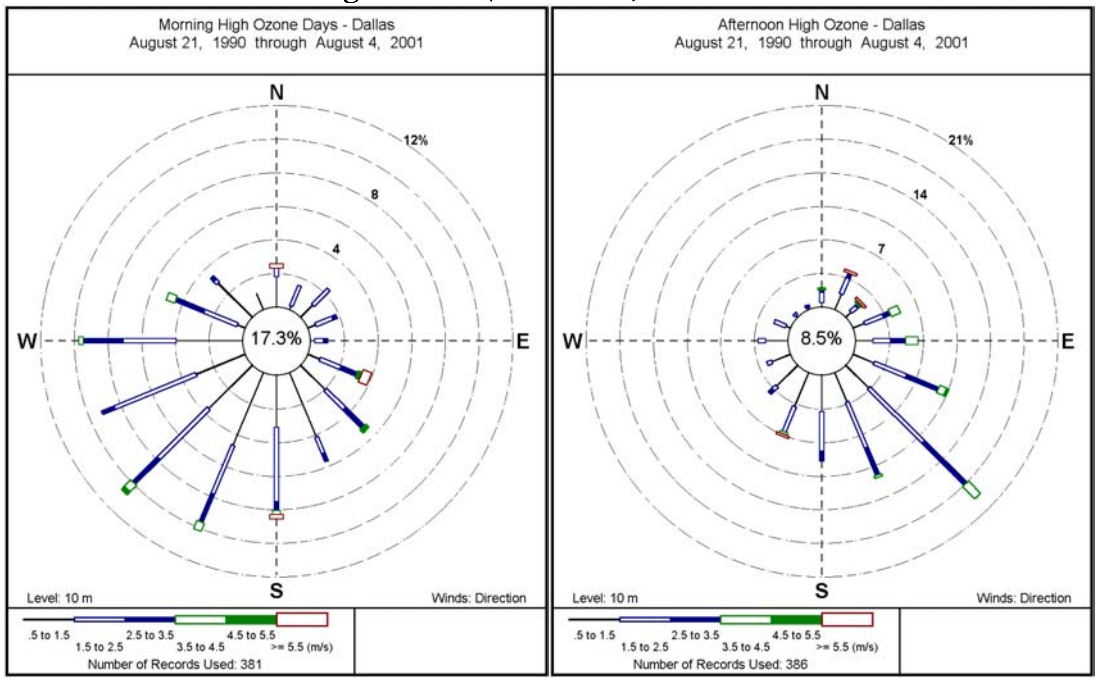


Figure 2-12. Surface wind roses for Dallas high ozone days 1990-2001 (TCEQ).

Low Ozone (O3 < 80) for Dallas

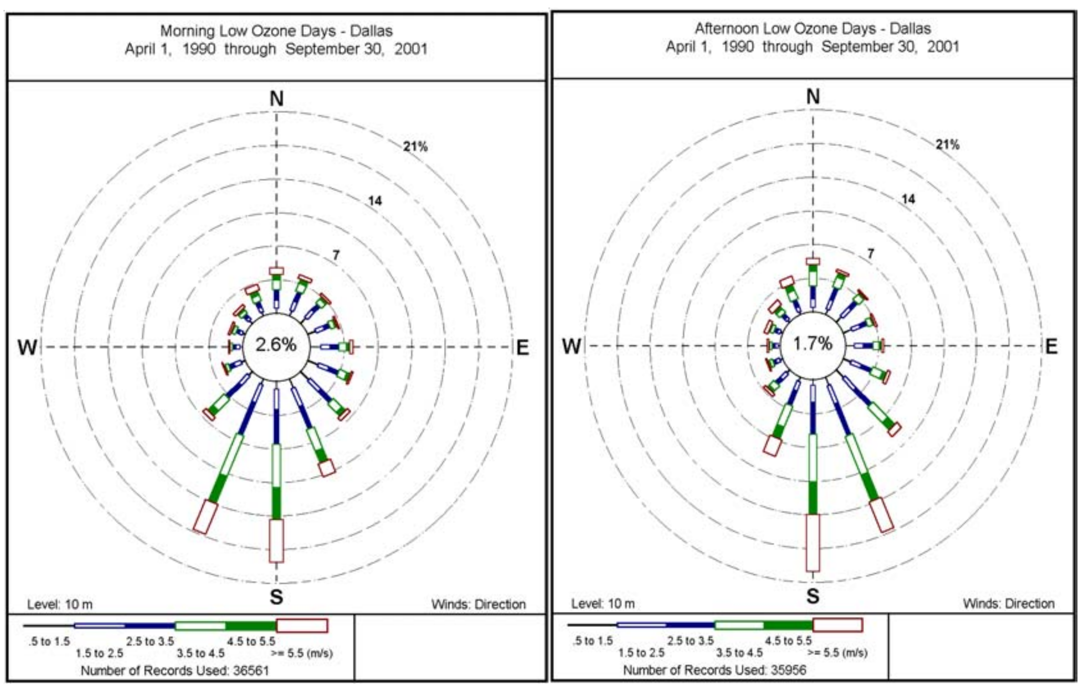


Figure 2-13. Surface wind roses for Dallas low ozone days 1990-2001 (TCEQ).

High Ozone (O3 > 125) for Fort Worth

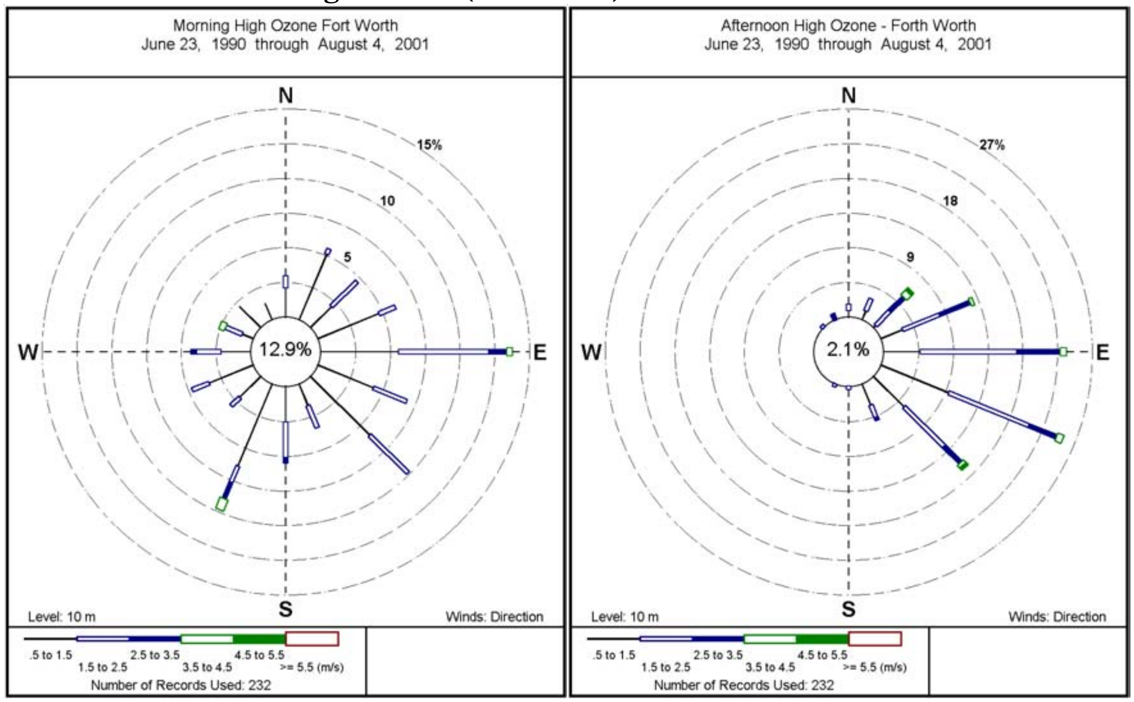


Figure 2-14. Surface wind roses for Fort Worth high ozone days 1990-2001 (TCEQ).

Low Ozone (O3 < 80 ppb) for Fort Worth

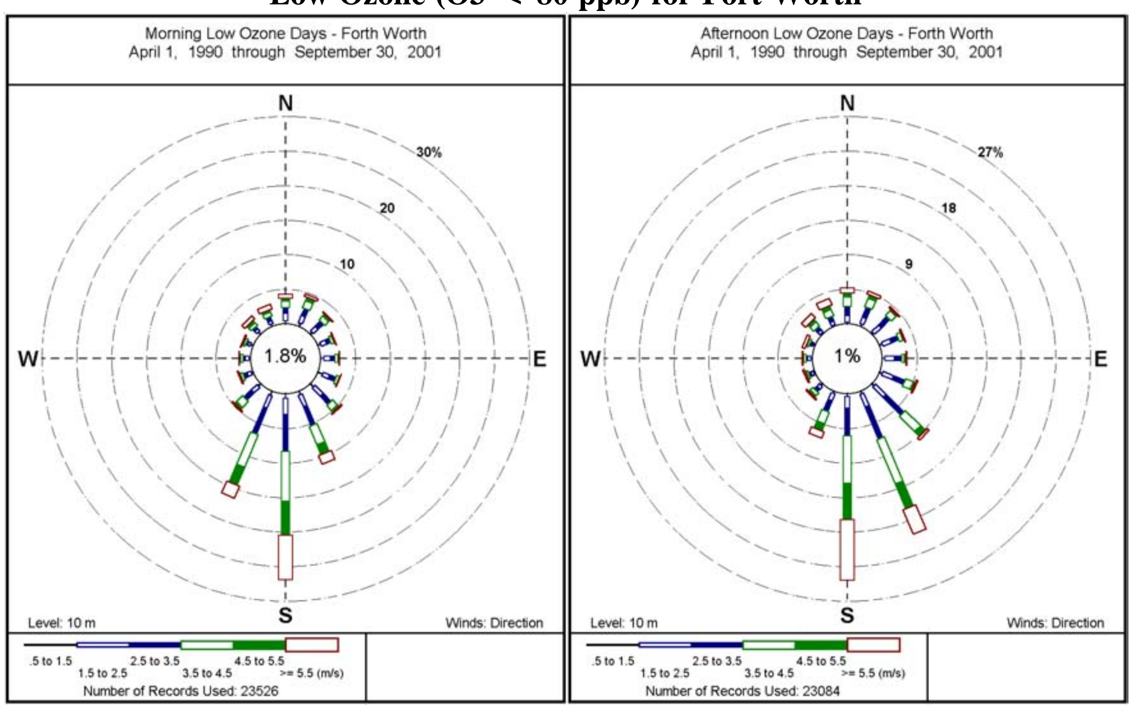


Figure 2-15. Surface wind roses for Fort Worth low ozone days 1990-2001 (TCEQ).

Regional Transport

An analysis of upper level winds provides information concerning the effects of long-range, or regional, transport on ozone levels within the DFW non-attainment area. NOAA's Air Resources Laboratory HySplit model was used to compute backward trajectories for air masses terminating in the DFW area. In addition, analyses of National Weather Service (NWS) weather maps were conducted in order to further characterize meteorology typical of the peak ozone seasons (June/July and August/September) in the DFW area.

Based on analyses of NWS weather maps the following observations concerning high ozone events in Texas can be made. High ozone events occur when the air becomes stagnant, typically in the summer when temperatures are higher and when there are more hours of sunshine. In June and July of 1999, for example, the Bermuda High frequently sat offshore of Florida. The clockwise flow around the high often enhanced the afternoon sea breeze and produced thunderstorms, helping dilute ozone. Other times, the jet slid to the south to create a storm where the stronger winds near the front could dilute the pollutants.

In all of the high-ozone periods in August and September, the Bermuda High was outside the analyzed weather map domain. A slow-moving surface high could be found passing through the Northern Plains and Great Lakes, and the pressure gradients across Texas were very weak during most of these episodes. In the upper atmosphere, a ridge of high pressure over the central US was clearly defined on four of five high ozone events. Four events had 500mb heights over 5880m with the jet stream over Canada and weak upper level winds over Texas. The fifth period considered – September 15-21, 1999 – had heights near 5820m; the jet split near the west coast with the stronger branch staying in Canada while the weaker southerly branch headed eastward through all the southern states.

Figure 2-16 displays a back trajectory scatter plot developed as part of the conceptual model. Displayed are upper air back trajectories ending in the DFW area on all 1-hour and 8-hour ozone exceedance days during the years 1997 through 2002. The trajectories show the path an air parcel follows which originated the previous day. As can be seen, the wind trajectories tend to favor northeasterly, southeasterly and southerly directions. The trajectories on high ozone days generally do not come from the north and west.

Back trajectories ending in the DFW area associated with 1-hour exceedances during the years 1997 through 2002 are displayed in Figure 2-17. The preferred trajectory direction for 1-hour exceedances is seen to be easterly, southeasterly, and southerly.

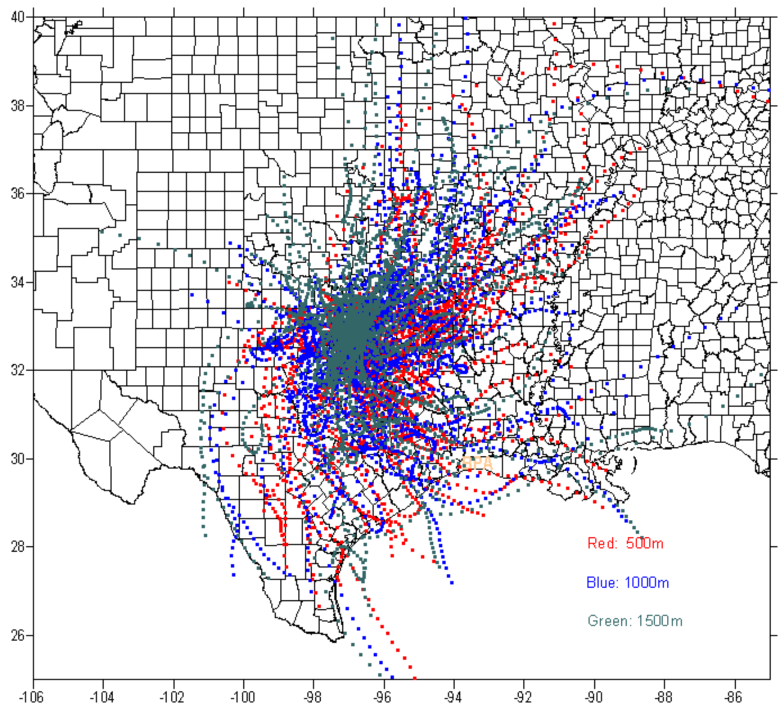


Figure 2-16. Back trajectory scatter plot on 1-hour and 8-hour ozone exceedance days during 1997-2002 in DFW. (TCEQ)

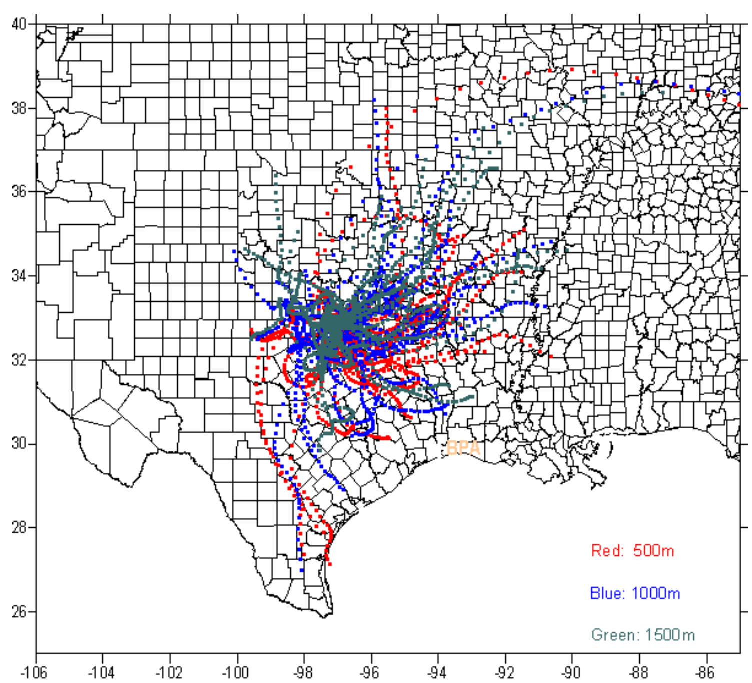


Figure 2-17. Back trajectory scatter plot on 1-hour ozone exceedance days during 1997-2002 in DFW. (TCEQ)

Back trajectories ending in the DFW area associated with 8-hour exceedances during the years 1997 through 2002 are displayed in Figure 2-18. The preferred trajectory directions for 8-hour exceedances are seen to be northeast, southeast and south.

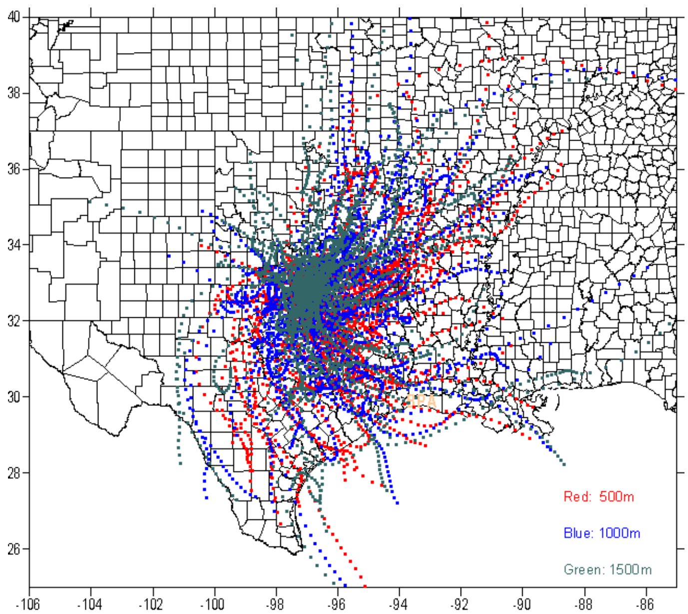


Figure 2-18. Back trajectory scatter plot on 8-hour ozone exceedance days during 1997-2002 in DFW.

Examination of Figures 2-16 and Figure 2-18 reveals that a significant number of trajectories originate in the upper Gulf Coast region, near Houston/Galveston and Beaumont/Port Arthur, particularly on 8-hour ozone exceedance days. A previous analysis completed by the TCEQ showed that approximately 13-22% of the time, the upper air trajectories originate from the Houston area. Trajectories which pass closer to Houston tend to have higher ozone and those which spend more time near Houston likewise have higher ozone levels. Thus, regional transport from the Houston non-attainment area has some effect on ozone air quality in the DFW region. This fact has implications for the 8-hour ozone standard as high regional ozone levels will potentially raise the background levels that contribute to high 8-hour ozone events.

As part of the development of the draft conceptual model for ozone formation in the DFW nonattainment area, the TCEQ performed statistical analyses on back trajectory data (TCEQ, 2002b). Figure 2-19 displays a statistical frequency plot for the DFW area. for the years 1993 through 1998. Examination of Figure 2-19 reveals that for trajectories originating near DFW (within 50 miles) the most frequent direction if from the southeast. For longer range trajectories (from 50 to 250 miles), the most frequent wind direction is from the south. Thus, the air quality in Dallas may be affected by sources in Houston since Houston sources may add to the background ozone concentration levels which are then transported long distances by upper air winds.

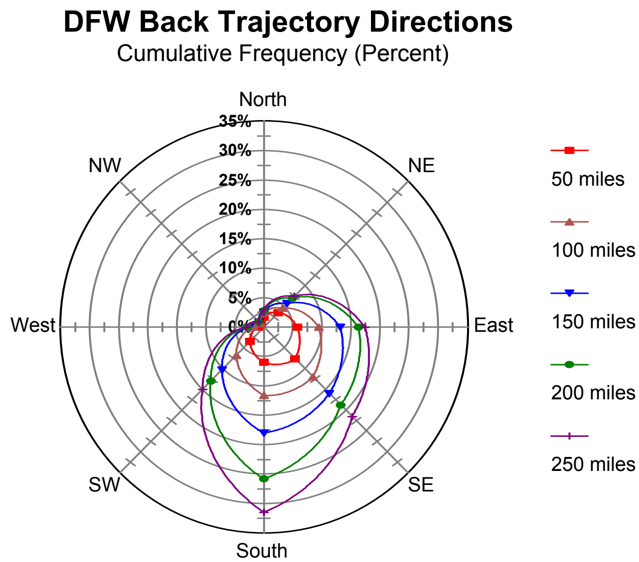


Figure 2-19. Back trajectory statistical frequency plot for DFW (TCEQ).

Evidence for long-range transport from Houston, as well as Beaumont/Port Arthur is further supported by previous analyses conducted by the TCEQ as part of the development of the draft conceptual model (TCEQ, 2002a; 2002b). A number of air quality model simulations were performed to investigate the potential for transport from the Houston/Galveston and Beaumont/Port Arthur nonattainment areas. The model simulations consisted of a number of experimental scenarios as well as source apportionment analyses.
The first assessment was based upon two previously modeled 8-hour ozone episodes (June 18-22, 1995 and June 30- July 4, 1996). Simulations were conducted in which anthropogenic emissions were zeroed out in various source regions and the modeling results were then evaluated to determine what, if any, impact was realized within the DFW non-attainment region. In the 1995 and 1996 zero out modeling the Houston plume was carried toward Austin and Tyler-Longview resulting in impacts of 2 to 10 ppb depending upon the episode day. The ozone impacts in the DFW area were relatively minor since the plume missed the DFW area. However, the modeling showed that Houston emissions could have a significant effect on the DFW area if the winds carried the plume in the correct direction.

In response to this finding, a special synthetic wind/zero out case was generated to determine the impact if winds blew directly from Houston to Dallas. These results indicated a plume of ozone reductions greater than 20 ppb stretching from northwest of Houston towards Dallas. In Fort Worth, ozone reductions of 5-10 ppb were realized, depending on the time of day.

Finally, Ozone Source Apportionment Technology (OSAT) was used to assess the contributions of various source regions on elevated ozone concentrations within the DFW area. These modeling results indicated measurable contributions from both the Houston/Galveston and Beaumont/Port Arthur non-attainment areas on the ozone maximums in DFW. The result of these analyses, as well as a more detailed discussion of the simulations performed may be found in TCEQ, 2000b.

2.6 EPISODE SELECTION

Based on the analyses conducted for the development of the conceptual model for ozone formation within the Dallas/Fort Worth non-attainment area, candidate modeling episodes were identified.

Previous Air Quality Modeling

The TCEQ has previously developed and modeled two ozone episodes for the Dallas/Fort Worth non-attainment area. These consisted of the June 18-22, 1995 and June 30 - July 4, 1996 episodes and were used for attainment demonstrations of the 1-hour ozone standard.

As pointed out previously, any new candidate episode should be relatively recent so that it represents the current emissions and be typical so its represents frequently occurring meteorological phenomena. New episodes should also satisfy the current 3-year design value window criteria. Finally, with the advent of the new 8-hour ozone standard, it is now desirable to develop episodes that would be useful for both 1-hour and 8-hour analysis.

The previously modeled 1995 and 1996 episodes both represented the most frequent transport direction, flow from the south and occurred during June/July, which was the secondary seasonal peak. The draft conceptual model and episode selection analysis reviewed several different candidate episodes that represent characteristics from missing time periods and/or transport directions. Thus the selection process considered episodes from the missing August/September seasonal peak ozone period and those representing transport from the east and/or southeast. However, some selected episode must represent transport from the primary direction.

Candidate Modeling Episodes

The selection and evaluation of candidate modeling episodes should be based on EPA guidance and also should consider the applicability and consistency with other non-attainment areas within the region. The draft conceptual model evaluated several possibilities from 1998 and 1999, as well as some possible 2000/2001 episodes. The goal was to select one or more episodes that could be utilized for both the 1-hour and 8-hour attainment demonstration and could be used to support photochemical modeling in other nearby areas.

All 1-hour and 8-hour exceedance days in the DFW nonattainment area from 1997 through 2002 were first identified from data obtained from the TCEQ. Back trajectory plots developed using the HySplit model were analyzed for each exceedance day to identify days associated with the primary transport directions. Preference was given to exceedance days and episodes that occurred during the primary ozone season (July, August and September). While the current focus is still on selection of 1-hour ozone modeling episodes, consideration was also given to periods that also experienced 8-hour ozone exceedances.

Each of these preliminary episode periods was further evaluated with respect to EPA episode selection criteria. In addition, in accordance with EPA guidance, exceedance days occurring within the current 3-year design value period were given preference. Based on these criteria, a number of preliminary episodes were identified for further analysis. The preliminary episodes identified are as follows:

- August 25-27, 1997
- July 14-18, 1998
- September 1-5, 1998
- August 4-7, 1999
- August 13-22, 1999
- August 31 - September 5, 2000

Episode Selection

Based on the analyses conducted as part of the development of the conceptual model of ozone formation in the Dallas/Fort Worth nonattainment area and the EPA selection procedures, two candidate episodes from this field of six were selected as possible candidates for the 1-hour attainment demonstration air quality modeling in DFW. The candidate episodes are August 4-7, 1999 and August 16-21, 1999. The screening criteria used to reduce the field of six episodes down to two primary candidates were as follows:

- Both episodes occur during the seasonal peak ozone period of August/September;
- Both episodes represent previously un-modeled trajectory directions, transport from east southeast;
- Both have multiple 1-hour and 8-hour ozone exceedances in Dallas/Fort Worth;
- Both supported by robust meteorological data; and,
- Both occur during the last 3 years.

As it is desirable to replace the existing 1995 and 1996 episodes with a single modeling episode, the new candidate episode must also represent transport from the primary direction (i.e., flow from the South/Southeast). Further, the August, 4-7, 1999 episode had widespread thunderstorm activity, which complicates the meteorological modeling. Therefore, the August 16-21, 1999 episode became the primary candidate for 1-hour modeling. However, since the period surrounding the 1-hour exceedances is also a strong candidate for 8-hour modeling, the August 13-22, 1999 extended period was selected as the preferred modeling episode. Details of the final selection process are explained in the conceptual model (ENVIRON, 2002).

2.7 SUMMARY OF AUGUST 13-22, 1999 OZONE EPISODE

Table 2-1 shows the peak 1-hour and 8-hour ozone measured during the August 13-22, 1999 episode. The extended episode allows ramp up days for modeling and continues through the entire high ozone period. 1-hour exceedances occur four days during the middle of the period, and 8-hour exceedances occur nine out of the ten days of the episode.

Table 2-1. 1-hour and 8-hour exceedances during August 13-22, 1999 ozone episode.

Date	1-Hour Peak Ozone (ppb)	# 1-Hour Exceedances	8-Hour Avg Ozone (ppb)	# 8-Hour Exceedances
Aug 13, 1999	88	0	67	0
Aug 14	115	0	**103**	4
Aug 15	107	0	**97**	5
Aug 16	**127**	1	**107**	6
Aug 17	**150**	4	**126**	7
Aug 18	**131**	2	**116**	4
Aug 19	**128**	1	**108**	2
Aug 20	108	0	**98**	1
Aug 21	111	0	**98**	5
Aug 22	101	0	**89**	3

Synoptic Analysis

Based on analyses of NWS weather maps, meteorology associated with this episode can be characterized as follows. Pressure gradients were very weak over Texas during the first four days. Winds were calm to 5 knots in the morning and southerly or easterly at 5-10 knots in the afternoon. Strong high pressure aloft and temperatures close to 100F on most days were recorded. Aloft, pressure was strongest during August 15-18, when the Dallas Ft Worth region was enclosed in a 5940m 500mb height contour with 10-20 knot winds. At the surface, a positively tilted 1023mb high was centered over the Great Lakes on August 15. To its east and south, a cold front stretched from eastern Maine to eastern Texas. As this high drifted eastward the next couple of days, a weak low followed, but stayed well to the north of Texas. On August 19, 500mb heights fell below 5940m, but stayed above 5880m through August 31. A 1011mb surface low was observed over southern Illinois on this morning with the associated cold front crossing the Dallas region around midday. Afternoon thunderstorms were detected near Dallas on that afternoon.

Behind this front, weak high pressure settled over the Great Lakes from August 20-22. Near Dallas, winds were north northeasterly following the frontal passage and then southeasterly late on August 21 and all day August 22. On August 22, Hurricane Bret made landfall near the southern tip of Texas. Clouds spread over Dallas on August 22 and 23, but precipitation was confined to its south and west.

Trajectory Analysis

Figures 2-20 a-j display the DFW back trajectories for the August 14-23, 1999 period. Long-range transport during the episode is seen to shift from the north, to northeast and to the southeast, reflecting the wind directions identified in the back trajectory analysis discussed in Figures 2-16, 2-17 and 2-18. Also considerable subsidence occurred during the period, which suppresses mixing and encourages accumulation of local emissions. Subsidence also reduces cloudiness, which allows more sunlight to reach the surface layers, increase temperatures and react with the local emissions to form ozone.

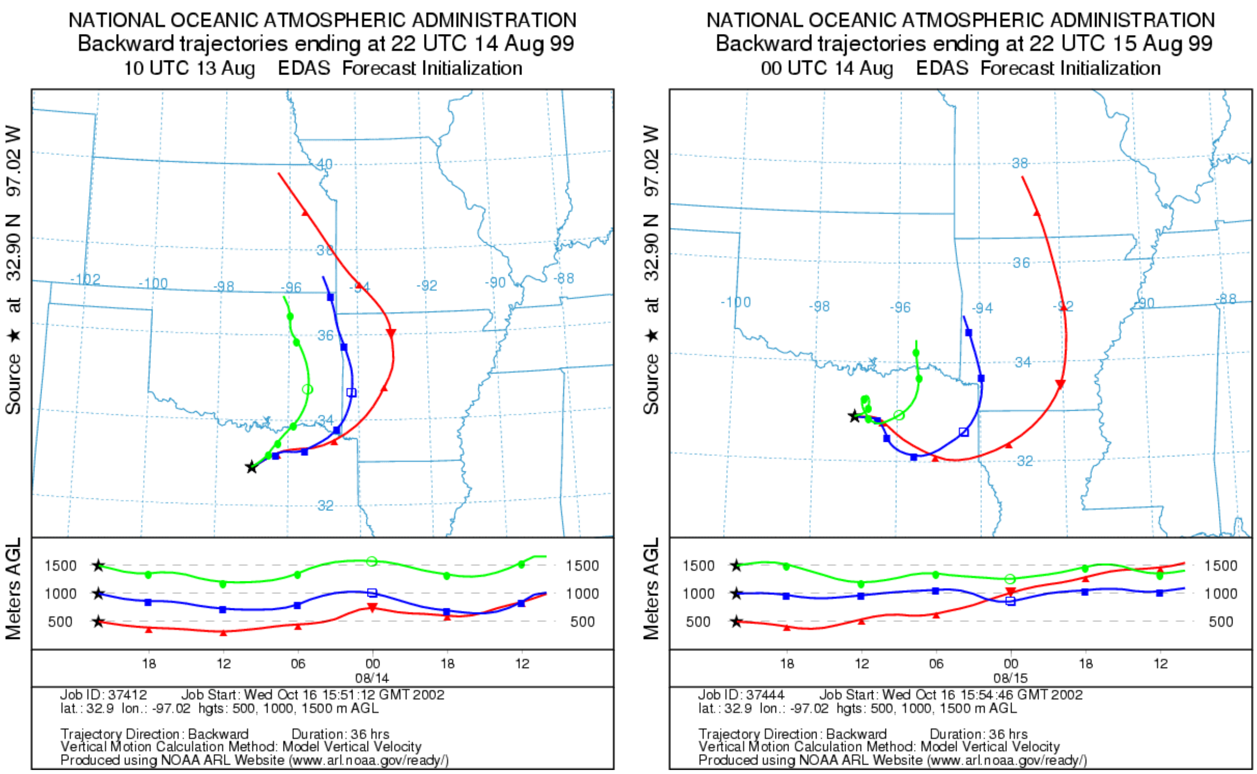


Figure 2-20 a-b. DFW back trajectories for August 14-23, 1999.

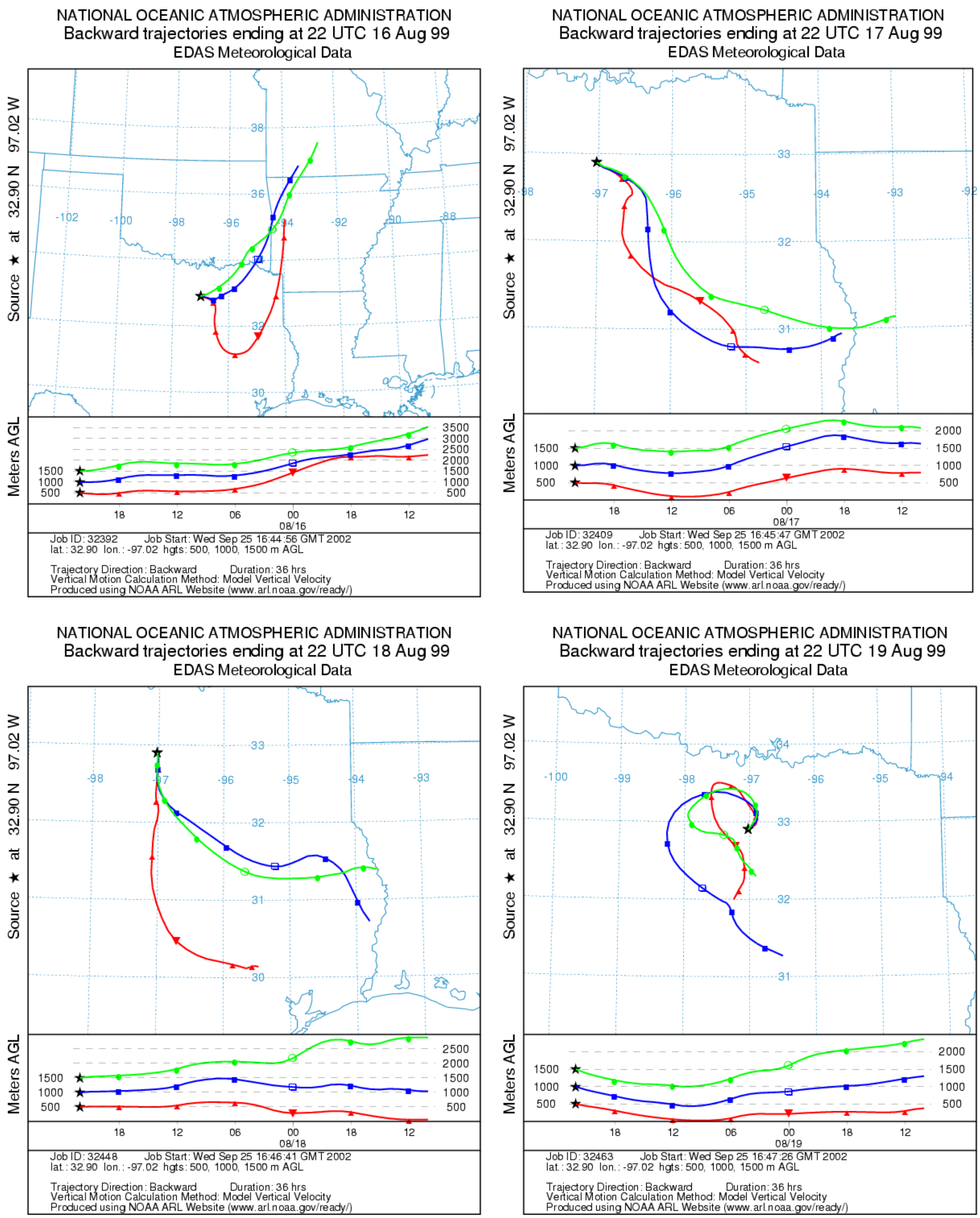


Figure 2-20 c-f. DFW back trajectories for August 14-23, 1999 continued.

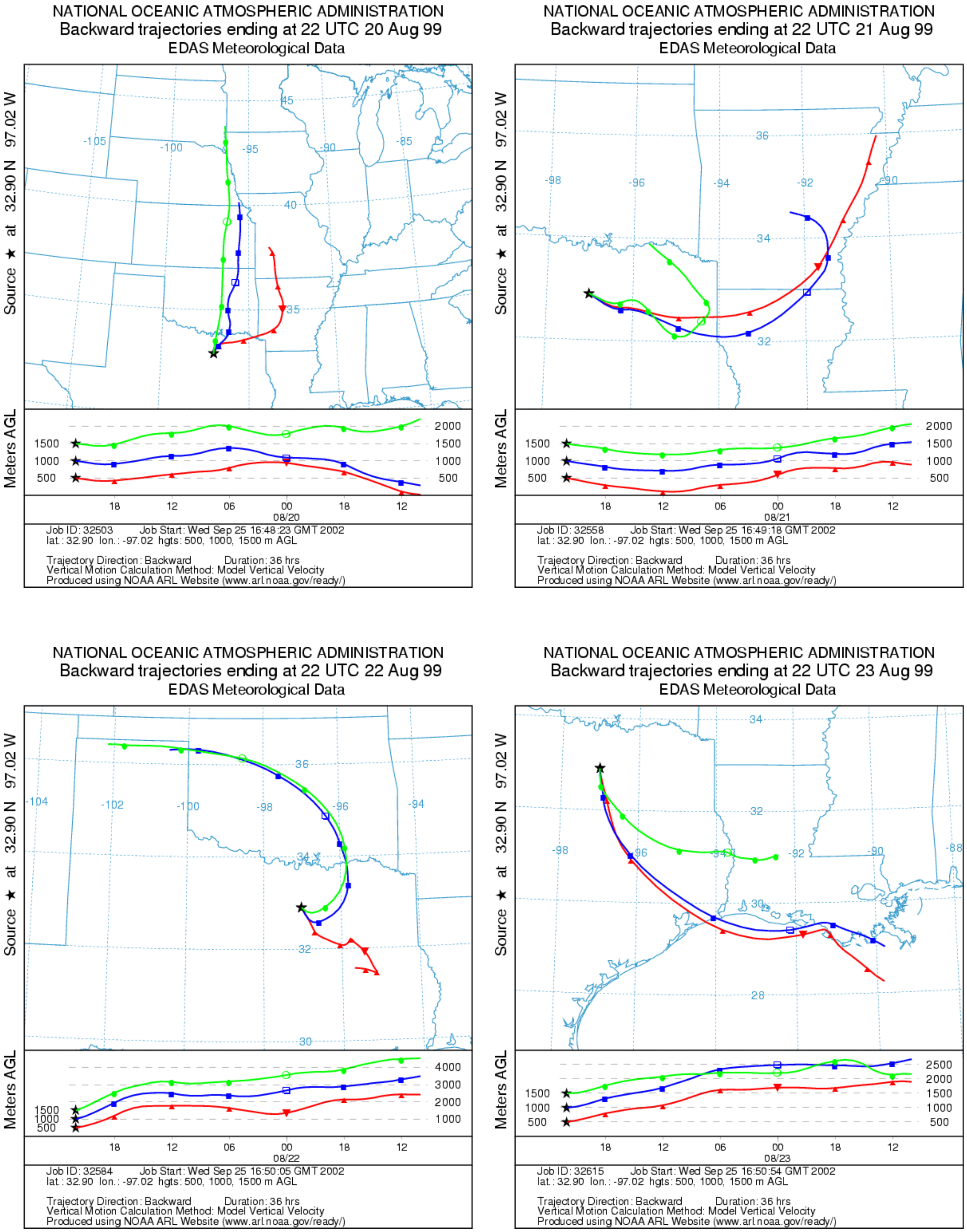


Figure 2-20 g-j. (Concluded). DFW back trajectories for August 14-23,1999.

Wind Speeds vs Ozone Concentrations

An analysis of local DFW surface winds and average monitored ozone concentrations in the area indicates that this episode is characteristic of typical conditions associated with elevated ozone concentrations. Figure 2-21 displays the average morning and afternoon surface wind speeds and ozone concentrations during the period August 13-22, 1999. Examination of Figure 2-21 reveals the relationship between surface wind speed and 1-hour and 8-hour ozone concentrations.

During the 1-hour exceedances period, August 16-19, 1999, wind speeds are seen to be very low and are inversely related to the peak 1-hour and 8-hour ozone concentrations. During the beginning and end of the episode, surface wind speeds are considerably higher, with correspondingly lower ozone concentrations. One-hour exceedances were measured on four days during the episode, with four monitors measuring exceedances on August 17th. The peak 8-hour average was also measured on August 17th, and 7 monitors exceeded the standard on that day.

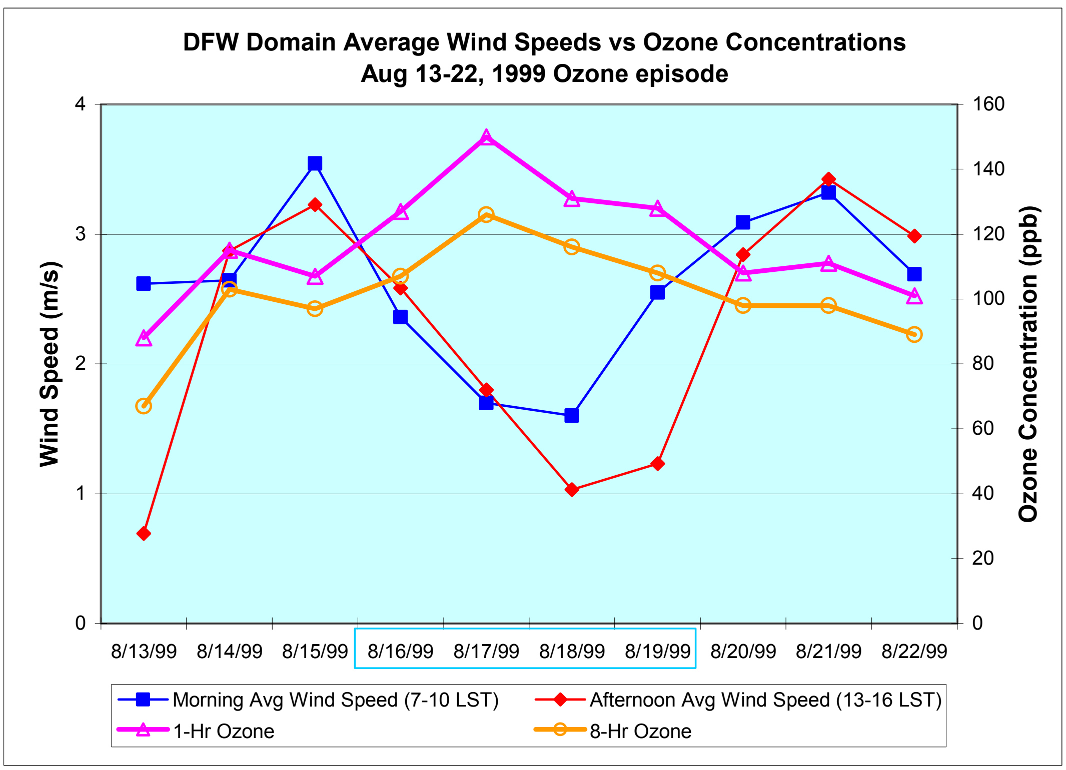
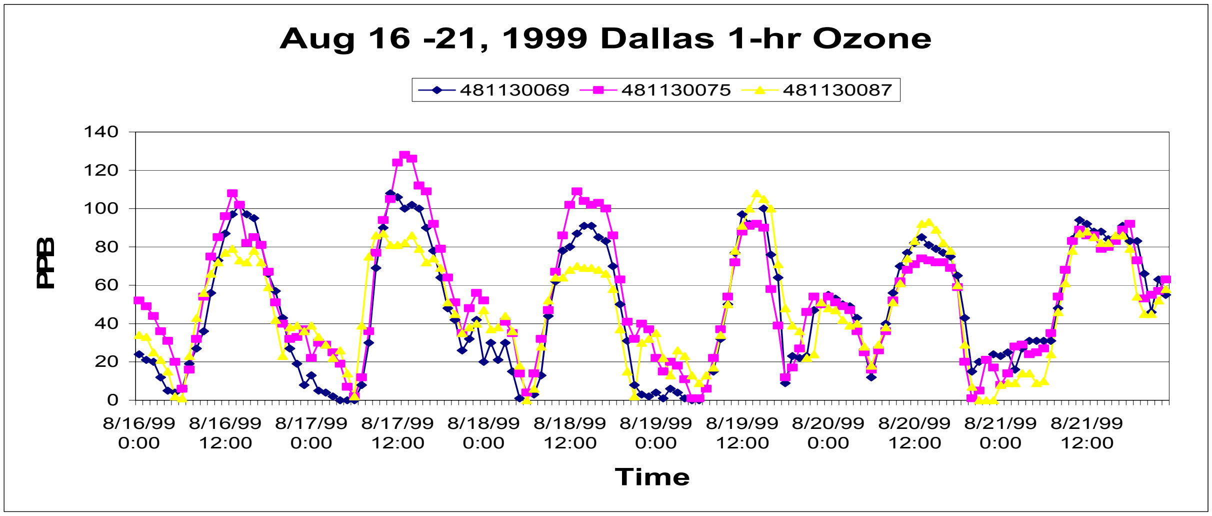
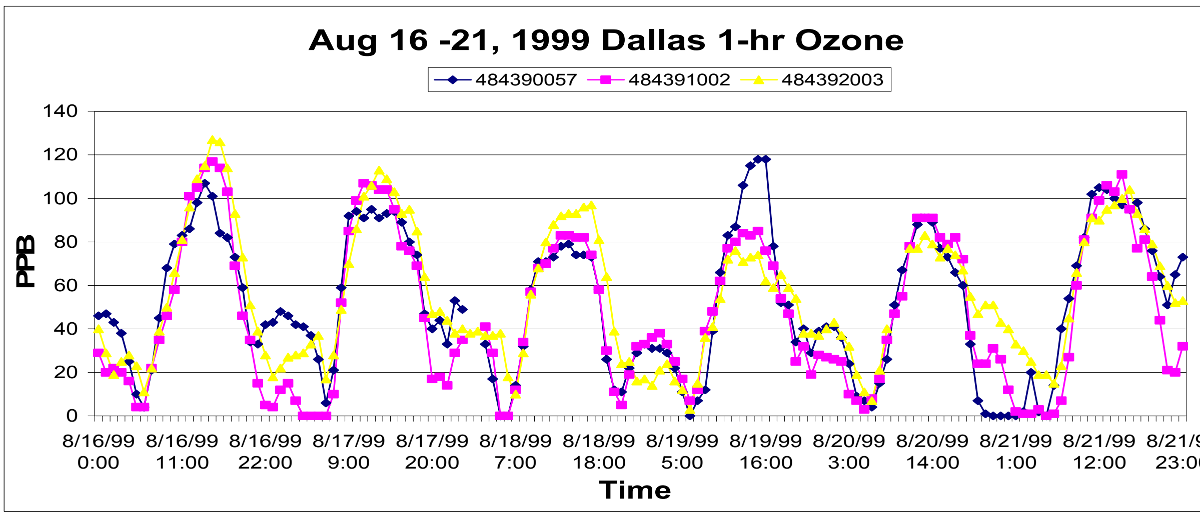


Figure 2-21. DFW domain average wind speeds and ozone concentrations (TCEQ).

Figure 2-22 shows the hourly time series of 1-hour ozone concentrations at monitors in the DFW area during the episode period.





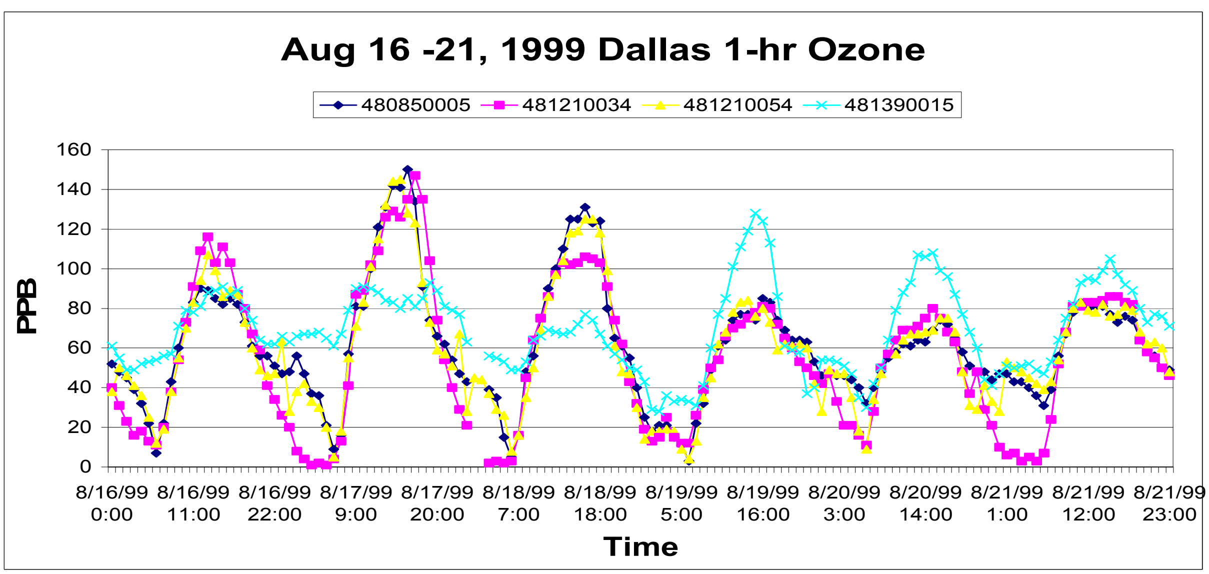


Figure 2-22. Time series of 1-hour ozone concentrations in DFW for August 16-21,1999.

Background Concentrations

The background concentrations were quite high during this episode averaging nearly 80 ppb during the 9 days with 8-hour exceedances. These relatively high background concentrations of ozone and precursors will affect DFW's ability to control the 1-hour and 8-hour ozone peaks occurring in the area. So an important part of this modeling effort will be to evaluate transport of ozone and precursors into the DFW area and the ability of the CAMx model to replicate the background concentrations.

Figure 2-23 shows the peak 1-hour and 8-hour ozone concentrations measured each day during the episode, as well as the background concentrations estimated each day. In this application we have defined the background concentration as the lowest peak ozone measured upstream of the DFW urban complex to reflect the ozone concentration that would have occurred if DFW had not added any emissions to the incoming air mass.

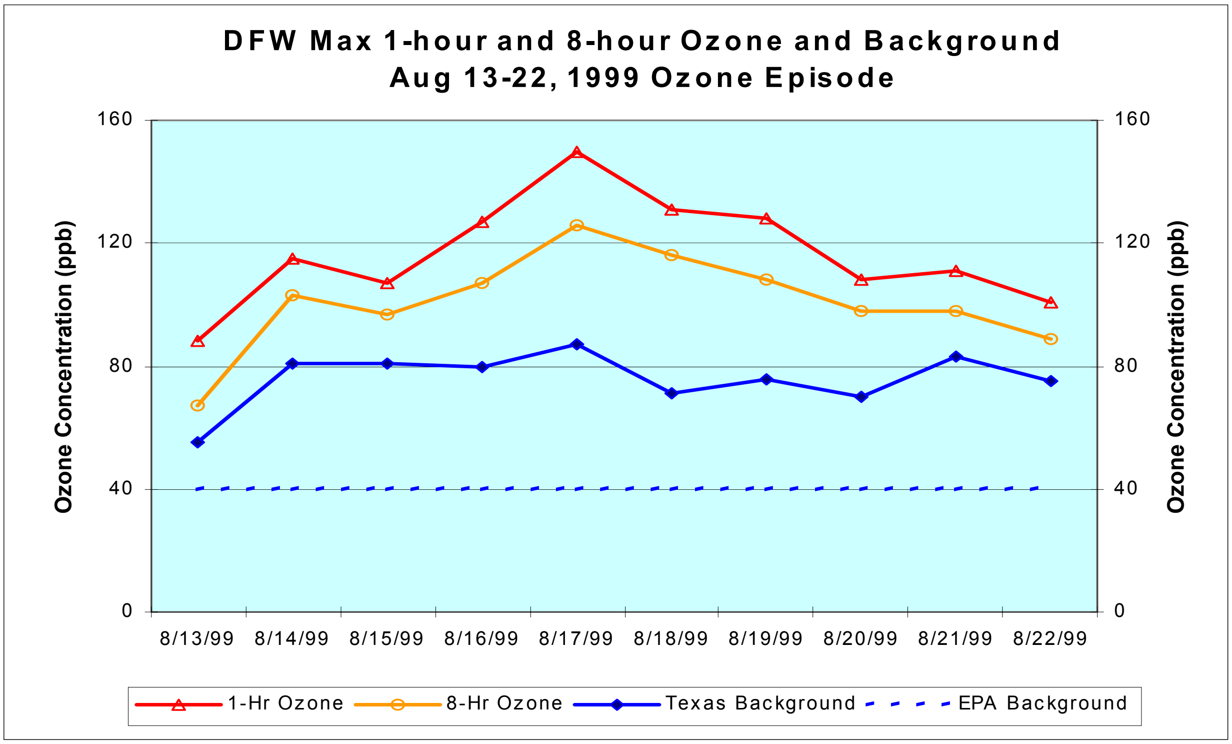


Figure 2-23. Ozone background concentrations during August 13-22, 1999 episode. (TCEQ).

Finally, it is important to point out that this episode is also being used for air quality modeling for the 8-hour ozone standard in East Texas. ENVIRON is currently modeling the TLM (Tyler/Longview/Marshall) area for the East Texas Council of Governments. The MM5 meteorological model has been applied for this time period with high resolution nested grids over both East Texas and the Dallas/Fort Worth areas. Thus, DFW may be able to take advantage of previous air quality assessments, emissions inventory, and meteorological modeling completed to date, including the experience gained from resolving issues and/or problems associated with the TLM modeling project.

3.0 MODEL SELECTION

This section introduces the models selected for use in the Dallas/Fort Worth 1999 Base Case Ozone Modeling Study and provides literature references to studies where the selected models have been evaluated and tested. The modeling methodology outlined in this protocol follows EPA's guidance for 1-hr regulatory modeling (EPA, 1991) as well as the draft guidance for 8-hr modeling (EPA, 1999) in ozone attainment demonstrations.

The models selected for this study include:

- The Fifth Generation PSU/NCAR Mesoscale Model (MM5, version 3.4) meteorological model (Dudhia, 1993)
- Version 2x of the Emissions Processing System (EPS2x) with the GloBEIS biogenic emissions processor
- The Comprehensive Air quality Model with extensions (CAMx, version 3.10) photochemical grid model (ENVIRON, 2000)

The logic and justification for these selections are as follows.

3.1 METEOROLOGICAL MODELS

Currently, the two most commonly used state-of-the-science prognostic meteorological models are:

- The Regional Atmospheric Modeling System (RAMS, version 4.3)
- The Fifth Generation PSU/NCAR mesoscale model (MM5, version 3.4).

A number of recent studies have compared the theoretical formulations and operational features of these models (see, for example, Mass and Kuo, 1998; Seaman, 1995, 1997; Pielke and Pearce, 1994). Other studies have evaluated their performance capabilities under a range of atmospheric conditions (e.g., Hanna et. al., 1998; Seaman et al., 1992, 1995, 1996; Tesche and McNally, 1993a-f; McNally and Tesche, 1996, 1998). Also, several studies actually present model performance evaluation results for the RAMS and MM5 models for the 1995 OTAG episode (Tesche and McNally, 1996; Tesche et. al., 1997). These studies reveal that MM5 and RAMS have very similar technical specifications and capabilities and can generate comparable performance in the hands of experienced practitioners.

RAMS

RAMS was originally developed at Colorado State University and is now a proprietary (but widely available) model that is continuously upgraded and maintained by Atmet. Similar to the MM5, the foundation of this model has evolved over a 20-year period. The current version of the RAMS model represents the blending of the Colorado State University Mesoscale Model (CSUMM), commonly referred to as the Pielke model (Pielke, 1974), and a non-hydrostatic cloud physics model (Cotton et al., 1982; Tripoli and Cotton, 1982). The SAIMM and CSUMM-FDDA (McNally, 1990) models are modest extensions of the early CSUMM code. RAMS has been used for several air quality studies, including the Lake Michigan Ozone Study, the OTAG modeling, regional ozone modeling for the state of Texas, and air quality modeling in El Paso.

RAMS is a limited-area prognostic meteorological model based on the full set of primitive dynamic equations govern atmospheric motions (Walko and Tremback, 1991). The equation set is non-hydrostatic with prognostic equations for wind components, temperature, moisture, and pressure. Optional parameterizations exist for turbulent diffusion; solar and terrestrial radiation; moist processes including the formation and interaction of clouds and precipitation; sensible and latent heat exchange between the atmosphere, multiple soil layers, and a vegetation canopy; the kinematic effects of terrain; and cumulus convection (Tremback et al., 1985). RAMS optionally incorporates a four-dimensional data assimilation (FDDA) package that nudges predictive fields toward gridded balanced objective analyses derived from meteorological measurements. This ability is particularly useful for historical air quality applications to minimize meteorological model error, or “drift”, in reproducing the conditions of the modeled episode.

In principal, the RAMS domain and grid cell sizes can encompass a broad range of scales, from microscale phenomena such as tornadoes and boundary layer eddies to large-scale synoptic systems. Two-way interactive grid nesting in RAMS allows local fine mesh grids to resolve compact atmospheric systems such as thunderstorms, while simultaneously modeling the large-scale environment of the systems on a coarser grid.

The model equations are solved horizontally on an Arakawa-C grid structure defined on a rotated Polar-stereographic map projection. The vertical coordinate is a terrain-following sigma-z representation. Typically, RAMS utilizes 30 or so vertical levels with the first grid point about 50 meters above the surface. The top of the model domain is typically around 16-km above sea level. Fine grids nested within this structure may have vertical resolutions as fine as 10 meters; the fine grid's top may be around 4-km above the surface. As many as four levels of grid nesting may be used. Prognostic equations are also used for the soil surface temperature and water content. The number of soil levels employed in RAMS is typically about a dozen in the top meter of soil. A uniform representative soil type is assumed for the full domain.

RAMS is available under license from Atmet. Current licenses fees range from zero for the Federal Government to about $10k with one year of technical support for other groups.

MM5

MM5 is the most technically advanced and widely used public-domain prognostic model. The model is described by Dudhia (1993). MM5 has been widely used for preparing inputs to urban- and regional-scale photochemical air quality models. EPA is using a version of the MM5 as part of the Models3 air quality modeling system.

MM5 was developed at Pennsylvania State University over 20 years ago, and in cooperation with NCAR, has consistently been improved and updated over the last 10 years. Like RAMS, MM5 is based on the full set of non-hydrostatic primitive equations. Optional parameterizations exist for boundary layer schemes; cloud and precipitation physics; heat budgets for multiple soil layers; the kinematic effects of terrain; and cumulus convection. MM5 can also encompass a broad range of scales, from the microscale to synoptic systems. One- or two-way interactive grid nesting is allowed, as well as moveable nests that allow the model to follow weather features such as hurricanes. MM5 also contains a FDDA package, but unlike RAMS, allows for nudging toward gridded analyses or individual observations separately or in combination.

The model equations are solved horizontally on an Arakawa-B grid structure defined on a number of available map projections. The Lambert Conformal projection is currently being used for large scale air quality applications in the U.S. The vertical coordinate is a terrain-following sigma-p representation. Typically, 20-30 vertical levels are specified, with the first grid point 20-50 meters above the surface, and the top of the model around 16-km above sea level.

MM5 is a publicly available at no cost and with no license restrictions.

Meteorological Model Selection

Either MM5 or RAMS would be technically appropriate for use in an ozone modeling study for DFW. For the DFW 1999 base case ozone modeling the MM5 meteorological model was selected because:

- It contains all of the technical attributes required to simulate meteorological conditions associated with 1-hour and 8-hour ozone exceedance events in the DFW area;
- It is publicly available to all with no license fees or restrictions on its use which allows industry and local governments to duplicate the modeling results.
- It is being used by the State of Texas for the development of several other ozone modeling projects including Houston and the Near-nonattainment areas.
- It is the meteorological model selected by CENRAP for regional haze modeling.

In this work, the latest version of MM5 (version 3.4) will be used.

3.2 EMISSIONS MODELING SYSTEMS

There are three main emissions modeling systems that are used to process anthropogenic emissions into the gridded, hourly resolved, and chemically speciated emissions needed for photochemical modeling.

EPS2: Version 2 of the Emissions Processing System was originally developed as part of the UAM-IV Modeling System (Morris and Myers, 1990). It is Fortran based and was designed to operate on 1990 era computer systems with memory constraints which limited its application to urban-scale modeling domains. More recently EPS has been speeded up and extended to treat regional-scale modeling domains (EPS2x). It is the emissions modeling system currently being used by the State of Texas for SIP modeling. It is Fortran-based, easy to use, and incorporates a strong quality assurance and reporting capability

EMS95/2000: The Emissions Modeling System (EMS) is a SAS-based emissions processor that was used extensively during OTAG. Since EMS is SAS-based and has strong quality assurance capability, emissions summary reports can be easily prepared and checked. The main weakness of EMS is that it requires a SAS license, some user expertise in SAS, and that it is slower than the Fortran based models.

SMOKE: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is a Fortran based system that is faster than the other two emissions models. However, the quality assurance (QA) is not integrated into the model as well as the other two systems. Recent experience in the Western Regional Air Partnership (WRAP) in which SMOKE was applied by its developers, suggests that the QA weakness in SMOKE caused numerous difficulties that would be difficult to overcome when preparing a SIP under a tight schedule.

The GloBEIS model is used to develop biogenic emissions estimates instead of SMOKE-BEIS or BEIS-3 because GloBEIS offers several advantages over these other models. The key advantages of GloBEIS are: updated (1999) emission factors; ability to incorporate detailed landuse data; ability to use solar radiation data from GOES satellite imagery; as well as built in QA and reporting functions.

Emissions Model Selection

In selecting an emissions modeling system for DFW ozone modeling, the following criteria were considered:

- Ability to incorporate EPA's MOBILE6 and NONROAD emissions estimates into the modeling system.

- Fast processing of emissions to generate model-ready inventories.

- Strong Quality Assurance (QA) and reporting capabilities.

- Free public access and availability without any restrictions on its use.

- Compatibility with other previous and ongoing work in other areas.

EPS2x was selected as the preferred emissions modeling system because it was the only model that satisfied all of the criteria above. Texas also has considerable experience with EPS2x since it is currently being used by the State of Texas in other SIP modeling.

Note that use of the SMOKE emissions modeling system was strongly considered, as that is the direction EPA is heading and it will also likely be used by CENRAP in the future. However, our experience with SMOKE in the WRAP modeling is that some features are still under development and testing. Further, the Quality Assurance (QA) component is not as advanced as either EMS or EPS. Given the tight deadlines of the DFW ozone modeling activities, it was felt prudent to use a fully tested emissions model with strong QA/QC capability.

3.3 AIR QUALITY MODELS

Several photochemical air quality models have been developed for ozone modeling and applied to different areas in the U.S. EPA's latest draft Guidelines for Air Quality Models has no "preferred model," so areas can choose between several "alternative models." The latest EPA draft 8-hour ozone modeling guidance (EPA 1999) lists the following *prerequisites* for an alternative model to be accepted:

1. The model must not be proprietary.
2. It should have received a scientific peer review.
3. It should be applicable to the specific problem on a theoretical basis.
4. It should be used with a database that is adequate to support the application.
5. It should have performed in past applications in such a way that estimates are not likely to be biased low.
6. It should be applied consistently with a protocol on methods and procedures.

The following models have been used recently for SIPs:

UAM-IV: Version IV of the Urban Airshed Model (Morris and Myers, 1990) was developed by Systems Applications, Inc., and for many years was EPA's guideline model. However, EPA recently removed this guideline status in its draft revisions to the Modeling Guidance because the UAM-IV is now considered out-dated, although it continues to be used in a few areas mainly using older databases for continuity purposes (e.g., Los Angeles and the California SIP). Available from the EPA at http://www.epa.gov/scram001/.

CALGRID: The CALGRID model was developed by Earth Tech (www.src.com) and was originally funded by the California Air Resources Board (CARB) to improve upon the UAM. CALGRID has been used in the Massachusetts SIP. It is also an outdated model that is not currently being used for any SIP modeling.

UAM-V: Version V of The Urban Airshed Model was developed by Systems Applications International/ICF Consulting and has been used in the Georgia (Atlanta) SIP, by other states, and by the EPA. The public availability and proprietary status are unclear since license terms and availability depend upon who requests the model. A restricted license version of UAM-V is available from the EPA at http://www.epa.gov/scram001/ or the model can be requested from ICF Consulting.

SAQM: The SARMAP Air Quality Model was developed for the CARB and used for the California SIP. SAQM is available on request from the California Air Resources Board (ARB). It has not been used for any ozone SIP work outside of California and will likely be replaced soon in California by one of the newer nested-grid photochemical models (e.g., CMAQ and/or CAMx).

CAMx: The Comprehensive Air Quality Model with extensions was developed by ENVIRON and publicly available at www.camx.com. CAMx was used by the State of Texas for the Houston-Galveston, Beaumont-Port Arthur, and Dallas-Fort Worth ozone attainment demonstration modeling in the Texas SIPs. CAMx is also used by other states for their 1-hour and 8-hour ozone planning and by the EPA for the NOx SIP Call and other rulemakings.

MAQSIP: The Multiscale Air Quality Simulation Platform was developed by the North Carolina Super Computing Center and is publicly available at www.mcnc.org. MAQSIP was used for the North Carolina SIP. It was developed as a prototype for the EPA Models-3/ CMAQ model and is being superseded by Models-3/CMAQ.

CMAQ: The Models-3 Community Multiscale Air Quality (CMAQ) modeling system was developed by EPA as a “one atmosphere” model to address ozone, PM, and visibility issues within one modeling platform. It is only just beginning to be used and has not yet been applied for any SIP modeling.

The technical attributes of several available models are compared in Table 3-1.

Table 3-1. Comparison of several widely known ozone air quality models.

Model	CAMx	MODELS-3 CMAQ	MAQSIP	UAM-IV	UAM-V
Model Developer	ENVIRON	USEPA	MCNC	SAI	SAI
Computational Requirements	Medium	High	High	Medium	Medium
Documentation	Good	Good	Good	Good	Good
Ease of Use	Fair	Poor	Fair	Fair	Fair
Availability	Publicly Available	Publicly Available	Publicly Available	Publicly Available	Restricted
Horizontal Advection	PPM, Bott, Smolarkiewicz	PPM, Bott	Bott, Smolarkiewicz	Smolarkiewicz	Smolarkiewicz
Horizontal Diffusion	K-theory Varying Kh	K-theory Constant Kh	K-theory Constant Kh	K-theory Constant Kh	K-theory Varying Kh
Vertical Diffusion	K-theory Input Kv	Bulk and K-theory Internal Kv	Bulk and K-theory Internal Kv	K-theory Internal Kv	K-theory Input Kv

Model	CAMx	MODELS-3 CMAQ	MAQSIP	UAM-IV	UAM-V
Grid Nesting	2-way, 1-way	1-way	1-way	1-way	2-way, 1-way
Dry Deposition	Yes	Yes	Yes	Yes	Yes
Wet Deposition	Yes	Yes	Yes	No	Yes
Gas-Phase Chemistry	Updated CB4 SAPRC99	Updated CB4 RADM SAPRC99	CB4 RADM	CB4	Updated CB4
Plume-in-Grid	Yes	Yes	No	No	Yes
Source Apportionment	Yes (OSAT, APCA)	No	No	No	No
Process Analysis	Yes	Yes	Yes	No	Yes
DDM Sensitivity Analysis	Yes	No	No	No	No

Final Selection of Photochemical Air Quality Model

In selecting an air quality model for ozone modeling of DFW, the following technical capabilities were considered important:

- Two-way grid nesting is essential for regional scale modeling in order to accurately depict fine scale local ozone formation in the Dallas and Fort Worth areas as well as characterizing ozone transport for upwind regions. One-way grid nesting is considered inadequate because emissions are not treated consistently between the coarse and fine grids.

- A plume-in-grid algorithm is required to adequately represent the strong gradients and ozone chemistry near major NOx sources.

- An updated chemical mechanism is required. The minimum standard is considered the Carbon Bond IV mechanism with updated radical termination reactions and updated isoprene chemistry as used in the OTAG modeling.

- Updated transport algorithms with low numerical diffusion are highly desirable to accurately represent plume impacts of major sources. The PPM or Bott advection schemes are state-of-the-science whereas the Smolarkiewicz scheme is out-dated.

- Free public access and availability without any restrictions on use.

CAMx was selected as the air quality model for this study because it is the only model that satisfies all of the criteria listed above, is publicly available, has previously and is currently being used for several SIPs in other areas, and possesses numerous "probing" tools (e.g., source apportionment, process analysis and the direct decoupled sensitivity analysis). The State of Texas also has considerable experience with CAMx, and has used it successfully in the past for other SIP modeling in Houston/Galveston, Beaumont/Port Arthur, Dallas-Fort Worth, Tyler/Longview/Marshall and several near-nonattainment areas.

4.0 MODELING DOMAINS

An important step in the design of an ozone modeling system is specifying the domain and grid system. The ozone model (CAMx) domain is discussed first since most of the factors influencing domain selection pertain to the ozone model. Then the specifications for the meteorological modeling (MM5) domain are discussed. There is a close relationship between the CAMx and MM5 grids to ensure that meteorological information is transferred accurately from MM5 to CAMx.

The MM5 uses a Lambert Conformal Projection (LCP) grid system. CAMx can use multiple different grid projection systems including the LCP as well as others (e.g., UTM, Lat/long, and Polar Stereographic). In order to minimize any interpretation of the meteorological variables from MM5 to CAMx that could introduce mass inconsistencies it is preferred that CAMx use the same coordinate system as MM5. Thus, an LCP coordinate system will be adopted for CAMx.

4.1 LAMBERT CONFORMAL PROJECTION (LCP) DEFINITION

A Lambert Conformal Projection (LCP) horizontal grid coordinate system is defined by a latitude/longitude “center” (0-km, 0-km) point in the LCP grid, two latitude parallels (that are typical 30 and 60 degrees), and a grid origin offset from the “center” and the east-west and north-south extent of the modeling domain. The TCEQ has defined an LCP coordinate system for use in all current episode development in Texas (Houston/Galveston, Northeast Texas and San Antonio/Austin). For the DFW ozone modeling, the same LCP grid definition was adopted. The LCP coordinate system is defined with the central coordinate of the LCP grid at 100°W and 40°N with latitude parallels at 30N and 60N.

4.2 CAMx MODELING DOMAIN

The following factors were considered in defining the 4-km DFW CAMx air quality modeling grid:

- A high resolution (4-km) grid must exist over the key monitors within the Dallas/Fort Worth non-attainment area;
- The 4-km grid must be large enough to include local and nearby major sources of emissions;
- The regional domain must extend far enough upwind to include all sources that might contribute substantially to elevated ozone levels in DFW;
- The CAMx grid must closely match the MM5 grid to minimize distortion of the meteorological variables in transferring data from MM5 to CAMx.

These issues are discussed further below and a CAMx grid is recommended.

Horizontal Extent and Grid Spacing

EPA's draft guidance on applying models for 8-hr ozone (EPA, 1999) includes the following recommendations:

1. Use nested grids to conduct regional modeling;
2. The grid spacing over the receptor areas of interest should ideally be 4-5-km and should not be larger than 12-km;
3. Use a grid spacing of 36-km or less for the regional domain;
4. Make the regional domain large enough to include about a potential 2 day transport distance upwind of the area of interest.

Additional requirements follow from the selection of MM5 as the driving meteorological model coupled with the desire to closely match the CAMx and MM5 grids:

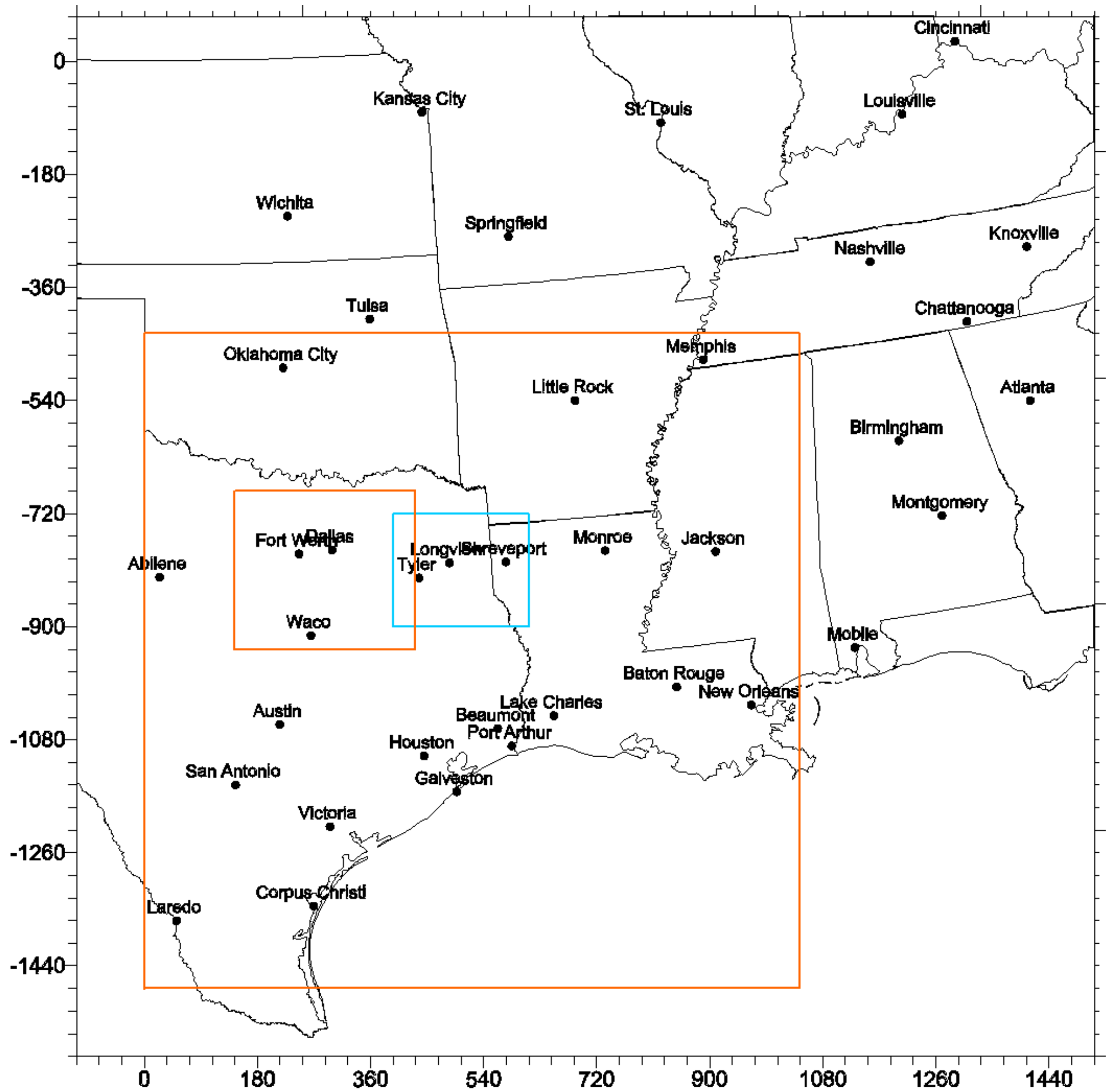
5. The grid spacings for the nested grids must be multiples of three (e.g. 36/12/4-km).
6. The grids must be defined in a Lambert Conformal Projection (LCP).

Based on all of these considerations, the CAMx grid for ozone modeling of DFW will use 4-km and 12-km fine grids nested within a 36-km coarse grid. The coordinate system for the grids will be Lambert Conformal Projection (LCP) with the central coordinate of the LCP grid at 100°W and 40°N. The CAMx domain is shown in Figure 4-1.

The 36-km and 12-km grids shown in Figure 4-1 are the same as for modeling Houston/Galveston, Northeast Texas and San Antonio/Austin. There are advantages of efficiency and consistency in having several modeling studies use a consistent grid system.

The 12-km grid includes all of the major upwind emission areas that may contribute to ozone transport into the DFW area under the most frequently occurring southerly wind episodes. In addition, the 12-km grid includes a substantial area that would be upwind of DFW during an ozone episode with other transport directions. This is important to accurately represent any influence of ozone transport since ozone formation is modeled more accurately by a 12-km grid than a 36-km grid. The intention is to accurately model potential transport of ozone from areas at a distance upwind of about 2 days transport.

A single 4-km grid covers the DFW non-attainment area and includes all the emission sources in the immediate vicinity of the urban areas. The 4-km domain extends north to the Texas/Oklahoma border and south to include the Waco urban area. The DFW 4-km modeling domain is shown in Figure 4-1. Also shown in Figure 4-1 is the 4-km Tyler/Longview/Marshall modeling domain being utilized for the current CAMx modeling efforts in East Texas. Figure 4-2 displays details of the DFW 4-km modeling domain, including the location of the major urban areas in the region as well as the county boundaries, showing that all 12 counties in the DFW CMSA are included.



CAMx GRID DIMENSIONS
LCP Grid with reference origin at (40 N, 100 W)

36 km Grid:	45 x 46 cells	from	(-108, -1584)	to	(1512, 72)
12 km Grid:	87 x 87 cells	from	(0, -1476)	to	(1044, -432)
4 km Grid:	72 x 63 cells	from	(144, -936)	to	(432, -684)
TLM 4 km Grid:	54 x 45 cells	from	(396, -900)	to	(612, -712)

(nested grid dimensions do not include buffer cells)

Figure 4-1. CAMx 36/12/4-km nested grids for the 1999 DFW ozone modeling.

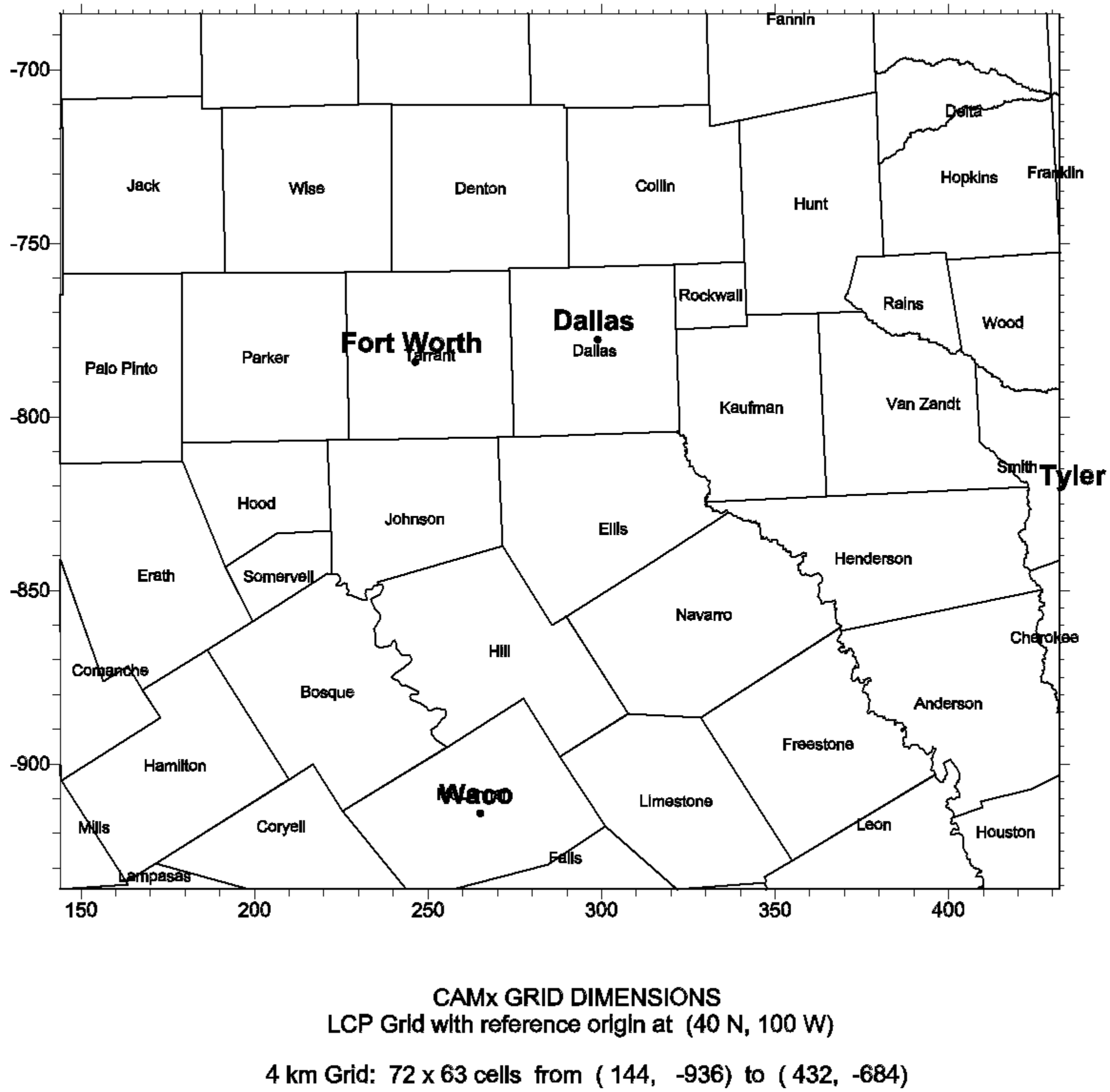


Figure 4-2. CAMx 4-km fine grid covering DFW for the August 1999 ozone episode.

Vertical Layers

EPA's current guidance on applying models for 8-hr ozone (EPA, 1999) includes the following recommendations on vertical layer structure:

1. Use 7-9 layers in the planetary boundary layer (PBL, the daily maximum mixing depth);
2. The surface layer should be no thicker than 50 m;
3. No layer within the Planetary Boundary Layer (PBL) should be thicker than 300 m; and
4. Add 1 or 2 layers above the PBL.

Under typical elevated ozone conditions in DFW the maximum depth of the PBL (i.e. mixing height) is about 2000 m AGL. The final CAMx layer structure will be determined when making the MM5 simulations, but the CAMx layer structure will be consistent with the EPA guidance and will have at least 10 layers up to a model top above 3000-m AGL. MM5 will have more layers than CAMx, and the CAMx layer interfaces will be matched to the MM5 layer interfaces to optimize the transfer of data from MM5 into CAMx. Figure 4-3 illustrates an example MM5 vertical layer structure and how CAMx would be configured with 15 vertical layers to match MM5 up to approximately 3500-m AGL. .

4.3 MM5 DOMAIN

The coarse and nested grids utilized in MM5 and CAMx will be defined on the same LCP projection and should completely match and overlay with the same resolution. However, the MM5 grids will be larger than the corresponding CAMx grids for the following reasons:

1. To remove any artifacts (i.e., numerical noise) that tend to arise in MM5 adjacent to fine grid boundaries; and
2. The extent of the coarsest MM5 grid will be much larger than the CAMx domain in order to provide a solid simulation of synoptic-scale meteorology (~1000's km, or continental scale) to the 36-km grid so that the simulation is not overly dependent on MM5 boundary conditions. In contrast, the coarsest CAMx domain needs to be sufficiently large to capture regional buildup of pollutants and 2-3 day transport to the receptors of interest (on the scale of multiple states).

The MM5 grids will be determined when the episodes are finalized. For MM5, the gridding arrangement will likely require a large master grid covering most of North America. As in many past modeling exercises, we will use a large 108-km coarse grid to feed to 36/12/4-km nested grids. We propose to use the MM5 data-assimilation package to nudge the MM5 predictions toward 3-hourly 40-km gridded meteorological analysis fields from the Eta Data Assimilation System (EDAS; described below). Therefore, the MM5 coarse domain is sized to fit within the spatial limits of the EDAS fields. In this case, the southern edge of the MM5 domain is pushed to the southern limit of the EDAS fields. This was necessary in order to model the flow over the entire Gulf of Mexico, and to provide sufficient room for all the nested grid boundaries in southern Texas and northern Mexico. The 36-km grid extends several grid points beyond the boundaries of the CAMx 36-km grid in each direction.

The 12-km MM5 grid will be placed over Texas, Louisiana, Arkansas, Oklahoma and Missouri to resolve larger mesoscale influences; it also is larger than the CAMx 12-km grid by several grid points (see Figure 4-1). Finally, the 4-km nested grid will cover the area of the CAMx 4-km grid with sufficient overlap that any boundary artifacts near the southern and western edges of the 4-km MM5 grid will not impact the CAMx grid.

In the vertical, MM5 will be configured to run with 28 levels, with a minimum surface layer depth of 20 meters, which will allow statistical comparisons between model output and surface measurements in the lowest layer of MM5. About ten layers will resolve the typical depth of the daytime boundary layer. The model will nominally extend to a pressure altitude of 100 mb (~16-km). Figure 4-3 displays one potential MM5 vertical layer configuration and a potential CAMx vertical layer matching to the MM5 vertical layer interfaces.

Once the MM5 modeling is complete and the performance is validated with the MetStat statistics program, the lowest surface layers may be consolidated for the CAMx modeling which will follow. In previous photochemical modeling exercises in Texas, consolidation has proven useful to prevent vertical mixing problems in the lowest layers of the atmosphere.

Layer	sigma	pressure	height	thickness	CAMx Layers
28	0.0000	50.00	18874.41	1706.76	
27	0.0250	73.75	17167.65	1362.47	
26	0.0500	97.50	15805.17	2133.42	
25	0.1000	145.00	13671.75	1664.35	
24	0.1500	192.50	12007.40	1376.75	
23	0.2000	240.00	10630.65	1180.35	
22	0.2500	287.50	9450.30	1036.79	
21	0.3000	335.00	8413.52	926.80	
20	0.3500	382.50	7486.72	839.57	
19	0.4000	430.00	6647.15	768.53	
18	0.4500	477.50	5878.62	709.45	
17	0.5000	525.00	5169.17	659.47	
16	0.5500	572.50	4509.70	616.58	
15	0.6000	620.00	**3893.12**	579.34	--15---
14	0.6500	667.50	**3313.78**	546.67	--14---
13	0.7000	715.00	**2767.11**	517.77	--13---
12	0.7500	762.50	**2249.35**	491.99	--12---
11	0.8000	810.00	**1757.36**	376.81	--11---
10	0.8400	848.00	**1380.55**	273.60	--10---
9	0.8700	876.50	**1106.95**	266.37	---9---
8	0.9000	905.00	**840.58**	259.54	---8---
7	0.9300	933.50	**581.04**	169.41	---7---
6	0.9500	952.50	**411.63**	166.65	---6---
5	0.9700	971.50	**244.98**	82.31	---5---
4	0.9800	981.00	**162.67**	65.38	---4---
3	0.9880	988.60	**97.29**	56.87	---3---
2	0.9950	995.25	**40.43**	20.23	---2---
1	0.9975	997.62	**20.19**	20.19	---1---
0	1.0000	1000.00	**0.00**		=============Surface======

Figure 4-3. Example MM5 vertical grid structure based on 28 sigma-p levels (including the surface). Heights (m) are above sea level according to a standard atmosphere; pressure is in millibars.

5.0 METEOROLOGICAL MODELING

The application of the MM5 meteorological model to prepare input fields for the ozone modeling is a complicated exercise that is governed by its own protocol. This section describes the general procedures that will be used in the meteorological modeling. It is understood that the application of a complex model like MM5 should not be undertaken using a prescriptive, pre-determined approach. Therefore, some model options and configurations may need to be refined during the project to improve model performance.

5.1 MM5 APPLICATION

We will operate the MM5 utilizing its Four Dimensional Data Assimilation (FDDA) capabilities. As a predictive (or forecasting) model, the MM5 is subject to a growing amount of error over the course of an extended simulation due to uncertainties in initial/boundary conditions, limits in spatial and temporal resolution, and simplifications in the governing equations. In simulations of historical episodes (as opposed to actual forecasting), FDDA is used to "nudge" model predictions toward observational analyses and/or discrete measurements to control model "drift" from conditions that actually occurred. This approach has consistently been shown to provide powerful advantages in running predictive mesoscale models for multi-day episodes, and has become a standard for photochemical applications.

For this project, we will supply the FDDA system with gridded meteorological analyses derived from the Eta Data Assimilation System (EDAS), which is archived at the National Center for Atmospheric Research (NCAR). Beginning in 1996, the EDAS provides 3-hourly gridded meteorological fields developed from the initialization cycle runs of the National Weather Service's Eta operational forecast model, which ingests observations from a combination of several systems (routine measurements from surface and upper air sites, radar networks, and satellite profilers). The EDAS domain covers most of the North American continent on a Lambert Conformal grid with 40-km grid spacing, and extends vertically from the surface to 50 mb (~20-km) with more than 20 pressure levels of data. We will augment this database with specialized data in the south-central U.S. to maximize performance in the areas of interest. These supplemental data include a wind profiler network (operated by the Forecast Systems Laboratory of NOAA), the EPA AIRS, observations from the Big Bend Regional Aerosol and Visibility Observation Study (BRAVO), which was operated in Texas between July and October 1999, and any local data available from Oklahoma.

The MM5 provides a wealth of options to configure the model for various parameterizations and physics packages. We will configure the model using the most appropriate options for each nested grid and for the meteorological conditions existing in the area of concern. A key MM5 option is which Planetary Boundary Layer (PBL) scheme to use. We are currently evaluating several schemes for applications in Texas and will consider the following PBL schemes for the DFW MM5 modeling.

- MRF
- Blackadar

- Gayno-Seaman TKE
- OSU
- Pleim-Xu

An initial MM5 run will be made that invokes the FDDA capabilities of the model, and that is configured with the physical treatments and options that, in our experience, have worked best in past photochemical modeling exercises. This configuration includes:

- FDDA analysis nudging of 3-hourly EDAS fields on the 108/36/12/4-km grids.
  - Above the boundary layer depth: MM5 will be nudged toward EDAS winds, temperatures, and humidity.
  - At the surface: MM5 will be nudged toward EDAS winds only, which will be augmented with routine and special observational wind data available in Texas during the episode.
  - In the boundary layer: we will rely on the latest MM5 boundary layer scheme to define the distribution of winds, temperature, and moisture up to 1-3-km above the surface.
- Simple-ice cloud microphysics will be employed for all grids.
- The Kain-Fritsch cumulus parameterization, which accounts for the effects of sub-grid scale convective activity, will be invoked for all grids except the 4-km nests.
- The Pleim-Xu boundary turbulence scheme will be employed for all grids.
- The cloud radiation scheme, which accounts for solar and terrestrial radiation impacts due to the presence of clouds, will be used for all grids.

Other MM5 configurations would be considered as needed, and we envision several additional MM5 runs would be made. The types of additional simulations issues may include:

- Observational (or point) nudging of surface and profiler wind observations in the 4-km grid (as opposed to analysis nudging).
- Intensity and level of observational nudging (i.e., which data to assimilate at what strengths).
- The impact of the size of the 4-km nested grid on the MM5 simulation.
- The impact of alternative cumulus parameterizations and boundary layer treatments.
- The impact of altering soil moisture contents.

Output from MM5 will be compared against meteorological observations from the various networks operating in Texas and throughout the south-central U.S. This will be carried out both graphically and statistically to evaluate model performance for winds, temperatures, boundary layer heights, and the placement, intensity, and evolution of key weather phenomena. The focus of this evaluation will center on performance in the 4-km grid. However, a regional analysis would also be carried out in different sections of the 12-km and 36-km MM5 domain. The problem with statistics is that the more data pairings that are summarized in a given metric, the better the statistics generally look, and so calculating a single set of statistics for the entire 36-km domain would not yield significant insight into performance. Therefore, a series of three to four sub-regional analyses of MM5 performance would be conducted. Results from the local and sub-regional evaluations should give clues as to any necessary modifications to be made in the MM5 configuration. .

5.2 GRID NESTING

Two-way nesting refers to the transfer of large-scale information down to nested grids, and the feedback of smaller scale influences up to larger grids. We will operate MM5 using two-way nesting for the 108/36/12-km grid simulation, and establish adequate model performance for the synoptic and larger-mesoscales before proceeding with the applications on the 4-km grid. However, we propose to operate MM5 using one-way nesting for the 4-km grid. In this approach, after the 108/36/12-km simulation is complete, 12-km grid results are extracted each hour to supply boundary information to the 4-km grid. Then MM5 is run separately for the 4-km grid, but the simulation results are not passed back to refine the 12-km results. This is a common practice among many mesoscale modelers. Our experience is that expansive 4-km MM5 simulations run quite slowly (even on our latest fast multi-processor machines), which severely limits our ability to run sensitivity tests if the complete 108/36/12/4-km grid system is run simultaneously. In our proposed approach, multiple MM5 runs for the 4-km nest can be made relatively quickly to optimize the model performance.

6.0 CAMx INPUT DATA PREPARATION

6.1 VERSION OF CAMx

The current publicly available version of CAMx is Version 3.10. An updated version of CAMx is expected to be released in early 2003. When made publicly available and if it does not interfere with the schedule we will migrate over to the latest version of CAMx.

6.2 EMISSIONS

CAMx requires two types of emission input files:

(1) Surface emissions from area, mobile, non-road, low-level point and biogenic sources are gridded to the CAMx nested grid system. This means that separate surface emissions files will be prepared for the 36 km, 12 km and 4 km grids. The surface emissions are injected into the lowest layer of the model.

(2) Elevated emissions from major point sources are injected into CAMx at the coordinates of each source. The plume rise for each source is calculated by CAMx from stack parameters so that the emissions are injected into the appropriate vertical layer. Emissions from selected major NOx emitters may be treated with the CAMx Plume-in-Grid (PiG) module.

The emission files will be prepared using version 2x of the Emissions Processing System (EPS2x). The emissions model must perform several tasks:

Temporal adjustments: Adjust emission rates for seasonal, day-of-week and hour-of-day effects.

Chemical speciation: Emission estimates for total VOC must be converted to the more detailed chemical speciation used by the Carbon Bond 4 (CB4) chemical mechanism in CAMx. Total unspeciated NOx emissions must be allocated to NO and NO_2 components.

Gridding: The spatial resolution of the emissions must be matched to the CAMx grid(s). Area sources are often estimated at the county level, and are allocated to the grid cells within each county based on spatial surrogates (e.g., population and economic activity). Mobile source emissions may be link specific (from transportation models) so links must be allocated to grid cells.

Growth and Controls: Emissions estimated for one year may need to be adjusted for use in a different year. In this project, the base year inventory may be for the same year as the modeling episode (1999) and so no adjustments will be needed. However, for 8-hour modeling it may be necessary to establish a different base year and adjust the emissions accordingly. At a later stage, future base inventories will also need to be adjusted for growth and controls anticipated in the attainment year.

Quality Assurance: The emissions model must have powerful QA and reporting features to keep track of the adjustments at each processing stage and ensure that data integrity is not compromised.

The outputs from the emissions model are called the "model-ready" emissions, and they are day-specific, gridded, speciated and temporally (hourly) allocated. EPS2x performs all of the processing steps for the anthropogenic emissions. The biogenic emissions are prepared using a different model (GloBEIS) because they are based on different input data and have specialized processing requirements (e.g., dependence on temperature, solar radiation and drought conditions).

Emissions Processing System (EPS2x)

The anthropogenic emission inventories will be processed using ENVIRON's enhanced version 2 of the Emissions Processing System (EPS2x). The original EPS2 was developed for EPA in the early 1990's. Design constraints imposed by the limited computer systems available at the time severely compromised performance for current regional modeling applications. However, EPS2 has all of the capabilities required for this study, and particular strengths of EPS2 include excellent reporting and QA capabilities and good documentation. ENVIRON has implemented several code revisions that greatly improve the speed of EPS2. With these modifications, the ENVIRON version of EPS2 has sufficient speed to perform the emissions modeling required for this project.

Anthropogenic Emissions Data Sources

The primary sources of emissions for the DFW ozone modeling study will be the NCTCOG (North Central Texas Council of Governments), TCEQ and the EPA. In the DFW CMSA and 4 km grid area, local data from the North Central Texas Council of Governments (NCTCOG) will be used. NCTCOG will conduct traffic demand modeling and develop day/hour specific link based emissions using the EPA MOBILE6 model. NCTCOG will also develop an offroad emissions inventory based on economic information, survey data, and the latest version of the EPA NONROAD model. Area sources in the 4 km grid area will be obtained from TCEQ.

TCEQ data will be the preferred data source for point sources and for onroad and nonroad emissions in Texas outside the 4-km grid. The most recent version of EPA's 1999 National Emissions Inventory (NEI) database will be used for most other states in the regional domain. Some data from the Louisiana Department of Environmental Quality (LA DEQ) will be used. The latest EPA emissions models will be used to estimate mobile source emissions, MOBILE6 for onroad mobile sources and NONROAD for offroad mobile sources.

Table 6-1 summarizes the source for emissions data that will be used in the DFW modeling.

Table 6-1. Summary of emissions data sources.

Category	Area	Data Source
Mobile	DFW	NCTCOG link-based, MOBILE6
	Texas major urban	TTI link-based, MOBILE6
	Other Texas	TTI county level, MOBILE6
	Outside Texas	EPA NET99, MOBILE6
Offroad	Texas	TCEQ, NONROAD model
	Outside Texas	EPA NET99 (area and offroad are combined)
Area	Texas	TCEQ
	Outside Texas	EPA NET99 (area and offroad are combined)
Point	TX and LA EGU	EPA acid rain hourly data processed by TCEQ
	Texas other	1999 PSDB
	Louisiana other	LA DEQ provided to TCEQ
	Other	EPA NET99
Offshore	Texas	TCEQ offshore and shipping emissions
Biogenic	Texas	GloBEIS3 with TCEQ LULC data and drought adjustment
	Outside Texas	GloBEIS3 with BELD3 LULC data

Biogenic Emissions

Biogenic emission inventories will be based on the most modern and scientifically advanced tool currently available, which is GloBEIS3. The State of Texas sponsored the development of GloBEIS through several projects performed by ENVIRON, the University of Texas at Austin, and the National Center for Atmospheric Research (NCAR). The GloBEIS model is publicly available at http://www.globeis.com along with a User's Guide and the report describing the model development. The key advantages of GloBEIS are: updated (1999) emission factors; ability to incorporate detailed landuse data; ability to use solar radiation data from GOES satellite imagery; and built in QA and reporting functions. The current version of GloBEIS is version 3. GloBEIS3 estimates the same emission levels as GloBEIS version 2.2 unless advanced features in GloBEIS3 (such as modeling the effects of drought or prolonged periods of high temperature) are employed. Biogenic emissions with/without drought conditions will be estimated using the advanced features of GloBEIS3 for sensitivity testing, but will be otherwise consistent with GloBEIS2.2.

Quality Assurance

Thorough quality assurance of the emissions processing is essential for this study to provide meaningful results. We will address this by setting up independent QA/QC procedures for each stage in the emissions processing. The primary QA/QC strategies will be as follows:

1. Review EPS2x log files from each processing step for error messages.
2. Track emissions totals through processing to ensure that data integrity is maintained.
3. Prepare emissions summary tables by source category.
4. Review emission density and tile plots prepared with PAVE and compare to LU/LC and vegetation data.
5. Evaluate day-to-day variation in emissions for consistency with expected changes due to temperature, day-of-week, etc.

6.3 METEOROLOGY

CAMx requires meteorological input data for the parameters described in Table 6-2.

Table 6-2. CAMx meteorological input data requirements.

CAMx Input Parameter	Description
Layer interface height (m)	3-D gridded time-varying layer heights for the start and end of each hour
Winds (m/s)	3-D gridded wind vectors (u,v) for the start and end of each hour
Temperature (K)	3-D gridded temperature and 2-D gridded surface temperature for the start and end of each hour
Pressure (mb)	3-D gridded pressure for the start and end of each hour
Vertical Diffusivity (m^2/s)	3-D gridded vertical exchange coefficients for each hour
Water Vapor (ppm)	3-D gridded water vapor mixing ratio for each hour
Cloud Cover	3-D gridded cloud cover for each hour
Rainfall Rate (in/hr)	2-D gridded rainfall rate for each hour

All of these input data will be derived from the MM5 results. MM5 output fields will be translated to CAMx-ready inputs using ENVIRON's MM5CAMx translation software. This program performs several functions:

1. Extracts data from MM5 grids and adjusts as appropriate to the corresponding CAMx grid.
2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers.
3. Diagnoses key variables that are not directly output by MM5 (e.g., vertical diffusion coefficients and cloud information).

The MM5CAMx program has been written to carefully preserve the consistency of the predicted wind, temperature and pressure fields output by MM5. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

The data prepared by MM5CAMx will be directly input to CAMx with the exception of the vertical diffusivity coefficients (Kv). Vertical diffusivities are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the photochemical model results are much more sensitive to diffusivities than the meteorological model results. We will evaluate the CAMx diffusion inputs by comparing several calculation approaches, and by analyzing available sounding data from profilers and rawinsondes. Based on prior experience, we may consolidate the first two layers of the MM5 modeling or apply minimum diffusivity values between layers 1 and 2 to ensure that nocturnal stability near the surface is not over-stated. The minimum value used will depend upon landuse (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

6.4 OTHER INPUT DATA

Initial and Boundary Conditions

The initial conditions (ICs) are the pollutant concentrations specified throughout the modeling domain at the start of the simulation. Boundary conditions (BCs) are the pollutant concentrations specified at the perimeter of the coarsest grid of the modeling domain. The boundary conditions will have little impact on the model results for DFW in this study because modeling is being performed over a large regional domain so the boundaries are far upwind from the cities of interest. One of the reasons for performing regional scale modeling with fine grid nesting (rather than small area urban scale modeling) is to minimize the importance of IC and BC estimates. Using a large regional domain moves the boundaries far away (in transport time and distance) from the study area. Including several "spin-up" days prior to the episode period also allows time for the model to generate its own ozone and reduce the influence of initial conditions.

Clean background values will be used for the ICs and BCs similar to the clean values used by the Ozone Transport Assessment Group (OTAG) for regional scale modeling of the Eastern US (OTAG, 1996). Changes from the OTAG values are the use of constant values of 40 ppb for ozone and 100 ppb for CO (Table 6-3). Previous modeling experience and numerous ozone measurements in Texas suggests that background concentrations of ozone are frequently as high as 60 ppb in many areas. However, the two day of spin-up time will allow the CAMx model to incorporate local emissions and bring background up to appropriate levels.

Table 6-3. Clean concentration values to be used for the initial and boundary concentrations (IC/BC).

Species	Concentration (ppb)
O3	40.0
NO	0.000049
NO2	0.08555
CO	100.0
PAR	3.078
HCHO	1.068
ETH	0.005315
ALD2	0.1051
TOL	0.006043
PAN	0.03834
HNO2	0.000728
HNO3	1.525
H2O2	2.263

Surface Characteristics (Land Use)

CAMx requires gridded land use data to characterize surface boundary conditions, such as surface roughness, deposition parameters, vegetative distribution, and water/land boundaries. CAMx land use files provide the fractional contribution (0 to 1) of eleven land use categories (Table 6-4) to the surface area of grid cell. Gridded geographic data will be developed from USGS landuse/landcover and topographic databases. Landuse data at 200 m resolution are freely available from a USGS web site for most of the nation.

Table 6-4. CAMx land use categories and the default surface roughness values (m) and UV albedo assigned to each category within CAMx.

Category Number	Land Cover Category	Surface Roughness (meters)	UV Albedo
1	Urban	3.00	0.08
2	Agricultural	0.25	0.05
3	Rangeland	0.05	0.05
4	Deciduous forest	1.00	0.05
5	Coniferous forest including wetland	1.00	0.05
6	Mixed forest	1.00	0.05
7	Water	0.0001	0.04
8	Barren land	0.002	0.08
9	Non-forested wetlands	0.15	0.05
10	Mixed agricultural and range	0.10	0.05
11	Rocky (with low shrubs)	0.10	0.05

Chemistry Data

Chemistry Parameters File

The CAMx "chemistry parameters" file determines which photochemical mechanism is used to model ozone formation. CAMx will be run with an updated version of the Carbon Bond 4 mechanism (CB4), referred to as mechanism 3 in CAMx, which is described in the CAMx User's Guide (ENVIRON, 2002). Mechanism 3 is the CB4 mechanism with updated radical-radical termination reactions and updated isoprene mechanism as used for the OTAG modeling and other previous TCEQ modeling studies.

Photolysis Rate File

The CB4 mechanism also includes several "photolysis" reactions that depend upon the presence of sunlight. The photolysis rates input file determines the rates for chemical reactions in the mechanism that are driven by sunlight. Photolysis rates will be calculated using the Tropospheric visible Ultra-Violet (TUV) model developed by the National Center for Atmospheric Research (Madronich, 1993 and 2002). TUV is a state-of-the-science solar radiation model that is designed for photolysis rate calculations. TUV accounts for environmental parameters that influence photolysis rates including solar zenith angle, altitude above the ground, surface UV albedo, absorption by aerosols (haze), and stratospheric ozone column.

Albedo, Haze and Stratospheric Ozone Column

The albedo/haze/ozone input file is used in conjunction with the photolysis rates input file to specify several of the environmental factors that influence photolysis rates. The photolysis rates and albedo/haze/ozone files must be coordinated to function together correctly. The surface UV albedo will be calculated based on gridded land use data using the land use specific UV albedo values given in Table 6-4. The albedo varies spatially according to the land cover distribution, but does not vary with time. The total ozone column will be based on satellite data from the Total Ozone Mapping Spectrometer (TOMS), which are available from a web site maintained by the NASA Goddard Space Flight Center (http://jwocky.gsfc.nasa.gov). Daily ozone column are available at 1.25°longitude by 1° latitude resolution and were mapped to the CAMx grid. The haze optical depth will be set to a clean regional value of 0.1.

6.5 CAMx MODEL OPTIONS

CAMx has several user-selectable options that are specified for each simulation through the CAMx control file. Most of these options follow naturally from other choices about model inputs. There are three main optional inputs that must be decided for this project: the advection scheme, the plume-in-grid scheme, and the chemistry solver. The recommended choices for these options are discussed below. See the CAMx User’s Guide (ENVIRON, 2002) for more details on these options. The selection for each option will be decided at the stage of the base case model performance evaluation and then held fixed for the remainder of the project.

Advection scheme: CAMx has three optional methods for calculating horizontal advection (the movement of pollutants due to horizontal winds) called Smolarkiewicz, Bott and Piecewise Parabolic Method (PPM). The Smolarkiewicz scheme has been used for many years, and was used in many previous studies in Texas with CAMx and the Urban Airshed Model (UAM). The Smolarkiewicz scheme has been criticized for causing too much artificial diffusion of pollutants, tending to "smear out" features and artificially overstate transport. The Bott and PPM schemes are newer and have less artificial diffusion than the Smolarkiewicz scheme. The Piecewise Parabolic Method will be used for this study since it has provided optimum results in previous work. Sensitivity to other advection options may be evaluated in the base case depending upon model results.

Plume-in-Grid: CAMx includes an optional sub-grid scale plume model that can be used to represent the dispersion and chemistry of major NOx point source plumes close to the source. We will use the Plume-in-Grid (PIG) sub-model for major NOx sources (i.e., point sources with episode average NOx emissions greater than 10 tons per day). Sensitivity to PIG treatment may be examined in diagnostic tests for the base case. A new version of CAMx is expected to be released in early 2003 that will have a more advanced PiG treatment, and may be evaluated if schedule permits.

Chemistry Solver: Starting with version 3 of CAMx there are two options for the numerical solution scheme for the gas phase chemistry. The first option is the CMC fast solver that has been used in every prior version of CAMx. The second option is an IEH solver. The CMC solver is fast and more accurate than most chemistry solvers used in current ozone models. The IEH solver is even more accurate than the CMC solver but significantly slower. Because of its speed, the CMC solver will be used for this study. Sensitivity to using the IEH solver may be examined in diagnostic tests for the base case if appropriate.

7.0 BASE YEAR MODEL PERFORMANCE EVALUATION

For the base year modeling, CAMx will be run for the August 13-22, 1999 episode and the performance of the model will be evaluated against available air quality data. The purpose of the evaluation is to build confidence in the model's reliability as an ozone prediction tool. The proposed evaluation plan will follow the procedures recommended in the EPA guidance documents for 1-hour ozone (EPA, 1991) and 8-hour ozone (EPA, 1999).

7.1 APPROACH TO MODEL PERFORMANCE EVALUATION

It is first important to establish a framework for assessing whether the photochemical modeling system performs with sufficient reliability to justify its use in developing ozone control strategies. The framework for assessing the model's reliability consists of the following principles, which are based on EPA's draft 8-hour modeling guidance:

- **The Model Should be Viewed as a System.** When we refer to evaluating a "model" we include not only the CAMx photochemical model, but its various companion preprocessor models (e.g., meteorological and emissions models) the supporting aerometric and emissions database, and all other related analytical and numerical procedures used to produce modeling results.

- **Model Acceptance is a Continuing Process of Non-Rejection.** Over-reliance on explicit or implied model "acceptance" criteria should be avoided, including EPA's performance goals (EPA, 1991). Statistical criteria are only the first step in evaluating model performance. Models should be accepted gradually as a consequence of successive non-rejections, and confidence builds as the model undergoes a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected.

- **Criteria for Judging Model Performance Must Remain Flexible.** This approach recognizes that the model can give the right answers for various combinations of wrong inputs. Statistical tests are a first step in the performance evaluation, but not in themselves final or definitive. The model output must also be compared to time series and geographical plots as well as precursor data when it is available. Performance may even be degraded as new information and procedures are inserted into the model, because new elements may illustrate the presence of compensating errors that were previously unknown.

- **Previous Experience is Used as a Guide for Judging Model Acceptability.** Interpretation of the CAMx modeling results for the episode, considered against the backdrop of the quality of the meteorological and emissions inputs and previous modeling experience will aid in identifying potential performance problems and suggest whether the model should be modified, tested further, or rejected.

Incorporating these principles into an operational philosophy for judging model performance, we suggest the following approach for assessing the reliability of the CAMx model for control strategy development. The model should produce peak unpaired ozone estimation accuracy, overall bias, and gross error statistics within the approximate ranges of ±15-20%, ±5-15%, and 30-35%, respectively. These performance standards have been established by the EPA for 1-hour ozone concentrations (EPA, 1991). EPA has not published any performance goals for 8-hour ozone, so the 1-hour ozone performance goals will be used to judge both 1-hour and 8-hour ozone model performance. If the model's performance is better than all of these ranges, the base case would not be rejected unless evidence from any supplemental diagnostic or sensitivity simulations suggest unusual or aberrant behavior.

If the base case fails any one of the above general ranges, it would become necessary to explain why the performance is poorer than commonly achieved in similar applications and whether the problems will compromise the evaluation of emission control strategies. An explanation or working hypothesis will enable developing appropriate diagnostic and sensitivity tests, and the possibility of bringing the model results into compliance. Without a working hypothesis to test, it is difficult to justify any changes to model inputs and the particular days (or base case) in question should be declared inadequate. After such an assessment, there are several potential courses of action: (a) diagnose the causes of poor performance and rectify the problems, or (b) eliminate the poor-performing episode (or a portion thereof) from use in strategy development and/or (c) identify an alternative episode for substitution in the study.

7.2 GRAPHICAL AND STATISTICAL EVALUATION

The evaluation of performance for the Dallas/Fort Worth 1-hour and 8-hour ozone modeling episode would be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level 1-hour and 8-hour ozone concentrations, and progressing to potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). The procedures outlined in the recent draft 8-hour modeling guidance illustrate the evolution in the EPA's previous 1-hour assessment procedures and provide a means by which to establish acceptable model performance:

1. Inspection of computer generated graphics, images and animations.
2. Calculation of ozone statistical metrics for bias, gross error and unpaired peak ozone.
3. Comparison of observed and predicted time series of precursor and intermediate species concentrations.
4. Comparison of observed and predicted ratios of indicator species.
5. Comparison of predicted source category contribution factors with estimates obtained using observational models.
6. Retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Sufficient fulfillment of these six points requires the availability of comprehensive measurement data on ozone and precursors from an extensive monitoring network. This may not be feasible in all cases, particularly in regards to the limited precursor measurements in the

DFW area. It is also quite possible that the list given above will change with the release of final guidance by EPA. Therefore, our proposed approach will consist of a blend of those points above and the three basic model performance steps outlined below. To the extent possible, each of the performance procedures described by EPA's 1-hour and 8-hour guidance will be addressed, and at a minimum, an explanation of why certain evaluations cannot be fulfilled will be provided (e.g., insufficient observational data).

Initial screening of the CAMx base case ozone predictions will be performed for the modeling episodes in an attempt to identify obviously flawed model simulations and to implement improvements to the model input files in a logical, defensible manner. If the screening phase suggests that no obvious flaws or compensating errors exist in the simulation(s), then the work will progress to the operational evaluation. The screening evaluation will employ ozone performance statistics, time series and tile plots. Graphical displays and animations will be generated using a combination of several common software packages that the ENVIRON team possess in-house, most of which are readily accessible to the project sponsors. These software packages include the Microsoft Excel, Surfer, and publicly-available PAVE. Examples of the types of graphical displays to be considered for each base case include:

- Ozone time series plots of predicted and observed hourly and 8-hour ozone;
- Ground-level 1-hour and 8-hour ozone isopleths compared to real world data;
- Ozone observed/predicted concentration scatterplots;
- Bias and error statistics stratified by for day of episode and sub-region.

Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. Any "curve-fitting" or "tuning" activity is to be avoided. The following principles should govern the performance improvement process (to the fullest extent possible given the modeling schedule):

- Any significant changes to the model or its inputs must be documented;
- Any significant changes to the model or its inputs must be supported by scientific evidence, analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred; and
- The TCEQ staff must review and approve any significant changes to the model or its inputs and advise the DFW Photochemical Modeling Technical Committee.

If the initial examination of the CAMx ozone output does not reveal obvious flaws, the formal operational evaluation follows. This activity consists of evaluation of ozone precursors and sensitivity/diagnostic simulations. Source Apportionment and Process Analysis techniques will allow evaluating the relative importance of source types and regions as well as evaluating the chemistry as it evolves in the CAMx model. Graphical displays and animations of Ozone, NOx and VOC data will be generated and compared to measured data where available. Note that for VOCs, it will only be possible to compare model performance for VOC species to the Hinton Drive monitor.

However, given the previous successful DFW modeling and knowledge that ozone in the area is primarily driven by mobile sources, it should be possible to examine the graphical displays for NOx and VOC at other locations for obvious flaws. Where previous modeling experience identifies discrepancies, additional model diagnosis and performance improvement efforts may be needed to fully identify, evaluate and correct the problems.

7.3 DIAGNOSTIC AND SENSITIVITY SIMULATIONS

Objectives

A limited number of diagnostic simulations will be performed to help understand and possibly improve base case model performance. In addition, sensitivity tests will be performed to diagnose model sensitivity to changes in key inputs. These tests are an important component of the base case model evaluation process. In general, diagnostic and sensitivity analyses serve to:

- Reveal model responses that are inconsistent with expectations or other model responses.
- Identify what parameters (or inputs) dominate (or do not dominate) model results.
- Examine the relationship between uncertainties in model inputs and model outputs (error propagation through the model).
- Identify alternate base cases that offer similar model performance and therefore identify potential compensating errors.
- Provide guidance for model refinement and data collection programs.

The exact number and nature of the sensitivity simulations that will be needed can only be assessed after the initial model performance evaluation is complete.

Tests That Are Not Recommended

With the advent of more sophisticated nested regional ozone models (such as CAMx) a number of sensitivity runs that were historically required by EPA guidance for the UAM-IV model are no longer needed or appropriate. These tests are zero-emission, zero initial condition, zero boundary condition runs and modified wind field tests such as halving the wind speeds. Physically unrealistic tests such as these can produce misleading results that are difficult to interpret. For the zero emission and zero IC/BC sensitivity tests, more can be learned from looking at sensitivity to alternate (but physically possible) inputs.

Ad-hoc, post processing modifications to wind fields outside of the meteorological models like MM5 are not recommended because they destroy consistency among the meteorological inputs (e.g., winds that are physically unrelated to pressures and temperatures). Other types of meteorological experiments such as alternate vertical eddy diffusivities or alternate vertical grid structures are potentially less destructive and may be more useful.

Recommended Tests

Sensitivity experiments will be considered as part of the performance evaluation analysis as appropriate. The potential need for and nature of these simulations will be discussed with the TCEQ staff in periodic telephone conferences and briefed to the Technical Review Committee as required. Up to 10 sensitivity/diagnostic CAMx simulations are planned.

Potential diagnostic evaluation runs include changes to:

- Boundary conditions, sensitivity of local background concentrations to more or less polluted boundary and initial conditions.
- Biogenic emissions, to evaluate sensitivity to uncertainties in biogenic emissions due to canopy temperatures and drought during the episode.
- PiG treatment, to check ozone sensitivity to the implementation of this submodel for sources in the lignite belt.
- Advection mechanism, to evaluate impact of this model option on performance.
- Meteorology, specific diagnostic tests identified during the preparation of the meteorological modeling such as: alternate vertical diffusion coefficients to adjust daytime and night time mixing heights toward observed data; impacts of clouds on photolysis rates; and impact of wet deposition.

Potential sensitivity runs include:

- Sensitivity to reductions/increases in total anthropogenic VOC and/or NOx emissions.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific source categories such as point, area, and mobile.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific urban areas and source regions (e.g., distant or local).

Use of CAMx Probing Tools for Diagnostic Evaluation

CAMx provides several "extensions" to the basic chemical/dispersion model, referred to as "probing tools", that provide information concerning source apportionment and the relative importance of various physical and chemical processes. These tools include the Ozone Source Apportionment Technology (OSAT and derivatives), the Integrated Process Rate Analysis Method (IPRAM), and the Decoupled Direct Method of tracking sensitivity coefficients to model inputs (DDM). All of these are described in the CAMx User's Guide for version 3.00 (www.camx.com).

For diagnostic purposes, the most useful tool is IPRAM, as this provides a wealth of information concerning the rates of change in ozone relative to transport and chemical processes. Reviewing this information can lead to insights into model performance and NOx/VOC-limited chemical kinetics in user-specified portions of the domain. Depending on project resources and schedule, use of IPRAM would be considered the primary tool for the diagnostic evaluation of the DFW CAMx Base Case simulations.

While OSAT and DDM would typically be used for assessing source apportionment for purposes of designing control strategy scenarios, both can be used in a diagnostic manner to assess the relative importance of various sources. In this way, the modeling team may be able to discover if a particular source area/category is having a stronger or weaker influence on ozone in key receptor areas than conceptually expected, and then undertake an investigation to determine if that response is appropriate or not. For understanding ozone contributions and identifying potential control strategy options, OSAT could be applied to generate source-receptor relationships. OSAT may be particularly useful for determining the level of ozone due to interstate and intrastate transport versus local sources in DFW.

REFERENCES

Dudhia, J., 1993. "A Non-hydrostatic Version of the Penn State/NCAR Mesoscale Model: Validation Tests and Simulation of an Atlantic Cyclone and Cold Front", *Mon. Wea. Rev.*, Vol. 121. pp. 1493-1513.

ENVIRON, 2002. Conceptual Model of Ozone Formation in the Dallas/Fort Worth Ozone Non-Attainment Area. Prepared for the Texas Commission on Environmental Quality. Prepared by ENVIRON International Corporation. October 16, 2002.

ENVIRON, 2001. Area and Mobile Source Emission Inventory Technical Support Project—1990-2010 Emission Inventory Trends and Projections. Prepared for the Texas Natural Resource Conservation Commission. Prepared by ENVIRON International Corporation, August 31, 2001

ENVIRON. 2002a. “User’s Guide to the Comprehensive Air Quality model with extentsions, version 3.10” available from www.camx.com. April.

EPA. 1991. “Guideline for Regulatory Application of the Urban Airshed Model”. EPA-450/4-91-013, U.S. Environmental Protection Agency Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. July 1991.

EPA. 1999. “Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS”. EPA-454/R-99-004. EPA Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. May 1999.

Hanna, S. R., et al. 1998. “Evaluations of Numerical Weather Prediction (NWP) Models from the Point of View of Inputs Required by Atmospheric Dispersion Models”, *5th International Conference on Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes*, 18-21 May 1998, Rhodes, Greece.

Madronich, S. 2002. The Tropospheric visible Ultra-violet (TUV) model web page. http://www.acd.ucar.edu/TUV/.

Madronich, S. 1993. “UV radiation in the natural and perturbed atmosphere”, in Environmental Effects of UV (Ultraviolet) Radiation (M. Tevini, ed.), Lewis Publisher, Boca Raton, pp. 17-69.

Mass, C. F. and Y. H. Kuo. 1998. “Regional Real-Time Numerical Weather Prediction: Current Status and Future Potential”, *Bulletin of the American Meteorological Society*, Vol. 79, No. 2, pp. 253-263.

McNally, D. E., 1990. "Incorporation of Four-Dimensional Data Assimilation into the Colorado State University Mesoscale Model", Project No. UCD201, Department of Land, Air, and Water, University of California, Davis, CA.

McNally, D. E. and T. W. Tesche. 1996. "Evaluation of the MM5 Model for the July 1988 and July 1995 Episodes and Comparison with the OTAG Meteorological Model, RAMS", to be presented at the *89th Annual Meeting of the Air and Waste Management Association*, 23-28 June 1996, Nashville, TN.

McNally, D. E. and T. W. Tesche. 1998. "Evaluation of the MM5 Meteorological Model Over the Greater Denver Front Range Region for Two Wintertime Episodes", prepared for the Denver Regional Air Quality Council, prepared by Alpine Geophysics, LLC, Golden, CO.

OTAG. 1996. "Modeling Protocol, version 3.0." Prepared by the Ozone Transport Assessment Group, 29 February, 1996.

Pielke, R. A. 1974. "A Three-Dimensional Numerical Model of the Sea Breeze over South Florida", *Monthly Weather Review*, Vol. 102, pp. 115-139.

Pielke, R. and R. Pearce, Eds. 1994. "Mesoscale Modeling of the Atmosphere", *Meteorological Monographs*, No. 47, American Meteorological Society, 156 pgs.

Seaman, N. L. 1995. "Status of Meteorological Pre-Processors for Air Quality Modeling", *International Conf. On Particulate Matter*, Air and Waste Mgt. Assn., Pittsburgh, PA.

Seaman, N. L. 1997. "Meteorological Modeling for Air Quality Assessments", NARSTO Critical Review Paper, 1998 NARSTO Ozone Assessment, to be submitted to *Atmospheric Environment*.

Seaman, N. L., et al. 1992. "The SARMAP Meteorological Model: A Four-Dimensional Data Assimilation Technique Used to Simulate Mesobeta-Scale Meteorology During a High-Ozone Episode in California", *International Specialty Conference on Tropospheric Ozone Nonattainment and Design Value Issues*, U.S. EPA/AWMA, 27-30 October, Boston, MA.

Seaman, N. L., et al. 1995. "A Multi-Scale Four-Dimensional Data Assimilation System Applied to the San Joaquin Valley During SARMAP. Part I: Modeling Design and Basic Performance Characteristics", *J. Appl. Meteo.*, Vol. 34, pp. 1739-1761.

Seaman, N. L., et al. 1996. "Application of the MM5-FDDA Meteorological Model to the Southern California SCAQS-1997 Domain: Preliminary Test Using the SCAQS August 1987 Case", *Ninth Joint Conference on Applications of Air Pollution Meteorology*, American Meteorological Society, 28 January-2 February, Atlanta, GA.

TCEQ, 2002a. Conceptual Model for Ozone Formation in the Dallas-Fort Worth Metropolitan, Draft Version 1.0, TCEQ, August 2002.

TCEQ, 2002b. Meteorological Factors Associated with 8-Hour Ozone Occurrences in the Dallas-Fort Worth Nonattainment Area, TCEQ, August 2002.

Tesche, T. W., et al. 1997. “Photochemical Modeling Analysis of the Pittsburgh-Beaver Valley Ozone Nonattainment Area: Volume IV -- Final Report”, prepared for the Southwestern Pennsylvania Stakeholders and the Pennsylvania Department of Environmental Protection, prepared by Alpine Geophysics, LLC, Covington, KY.

Tesche, T. W. and D. E. McNally. 1993a. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 1: 26-28 June 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1993b. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 2: 17-19 July 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1993c. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 3: 25-26 August 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1993d. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 4: 20-21 June 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1993e. "Operational Evaluation of the SARMAP Meteorological Model (MM5) for Episode 1: 3-6 August 1990", prepared for the Valley Air Pollution Study Agency, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1993f. "Operational Evaluation of the SARMAP Meteorological Model (MM5) for Episodes 2: 27-29 July 1990", prepared for the Valley Air Pollution Study Agency, prepared by Alpine Geophysics, Crested Butte, CO.

Tesche, T. W. and D. E. McNally. 1996. “Evaluation of the MM5 Model for Three 1995 Regional Ozone Episodes over the Northeast United States”, prepared for the Southwestern Pennsylvania Clean Air Stakeholders Group, prepared by Alpine Geophysics, LLC, Covington, KY.

Tremback, C. J., et al. 1985. "A Regional Scale Atmospheric Numerical Model Including Explicit Moist Physics and Hydrostatic Time-Split Scheme", *7th Conference on Numerical Weather Prediction*, Montreal, Canada. American Meteorological Society, Boston, Mass.

Tripoli, G. J. and W. R. Cotton. 1982. "The Colorado State University Three-Dimensional Cloud/Mesoscale Model: Part I: General Theoretical Framework and Sensitivity Experiments", *J. de Rech. Atmos.,* Vol. 16, pp. 185-195.

Walko, R. L. and C. J. Tremback. 1991. "RAMS: The Regional Atmospheric Modeling System", prepared by ASTeR, Inc., Fort Collins, CO.